Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJYC1621

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | AUG 06 | CAS REGISTRY enhanced with new experimental property tags |
| NEWS 3 | AUG 06 | FSTA enhanced with new thesaurus edition |
| NEWS 4 | AUG 13 | CA/CAplus enhanced with additional kind codes for granted patents |
| NEWS 5 | AUG 20 | CA/CAplus enhanced with CAS indexing in pre-1907 records |
| NEWS 6 | AUG 27 | Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB |
| NEWS 7 | AUG 27 | USPATOLD now available on STN |
| NEWS 8 | AUG 28 | CAS REGISTRY enhanced with additional experimental spectral property data |
| NEWS 9 | SEP 07 | STN AnaVist, Version 2.0, now available with Derwent World Patents Index |
| NEWS 10 | SEP 13 | FORIS renamed to SOFIS |
| NEWS 11 | SEP 13 | INPADOCDB enhanced with monthly SDI frequency |
| NEWS 12 | SEP 17 | CA/CAplus enhanced with printed CA page images from 1967-1998 |
| NEWS 13 | SEP 17 | CAplus coverage extended to include traditional medicine patents |
| NEWS 14 | SEP 24 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS 15 | OCT 02 | CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt |
| NEWS 16 | OCT 19 | BEILSTEIN updated with new compounds |
| NEWS 17 | NOV 15 | Derwent Indian patent publication number format enhanced |
| NEWS 18 | NOV 19 | WPIX enhanced with XML display format |
| NEWS 19 | NOV 30 | ICSD reloaded with enhancements |
| NEWS 20 | DEC 04 | LINPADOCDB now available on STN |
| NEWS 21 | DEC 14 | BEILSTEIN pricing structure to change |
| NEWS 22 | DEC 17 | USPATOLD added to additional database clusters |
| NEWS 23 | DEC 17 | IMSDRUGCONF removed from database clusters and STN |
| NEWS 24 | DEC 17 | DGENE now includes more than 10 million sequences |
| NEWS 25 | DEC 17 | TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment |
| NEWS 26 | DEC 17 | MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary |
| NEWS 27 | DEC 17 | CA/CAplus enhanced with new custom IPC display formats |
| NEWS 28 | DEC 17 | STN Viewer enhanced with full-text patent content from USPATOLD |
| NEWS 29 | JAN 02 | STN pricing information for 2008 now available |
| NEWS 30 | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

| | |
|---|---|
| NEWS HOURS | STN Operating Hours Plus Help Desk Availability |
| NEWS LOGIN | Welcome Banner and News Items |
| NEWS IPC8 | For general information regarding STN implementation of IPC 8 |

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:32:08 ON 25 JAN 2008

=> file reg

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 14:32:22 ON 25 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 24 JAN 2008 HIGHEST RN 1000773-19-2
DICTIONARY FILE UPDATES: 24 JAN 2008 HIGHEST RN 1000773-19-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\jcho2\My Documents\10588478.str

L1 STRUCTURE UPLOADED

=> dl1
DL1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d l1
L1 HAS NO ANSWERS
L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss full
FULL SEARCH INITIATED 14:33:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    79581 TO ITERATE

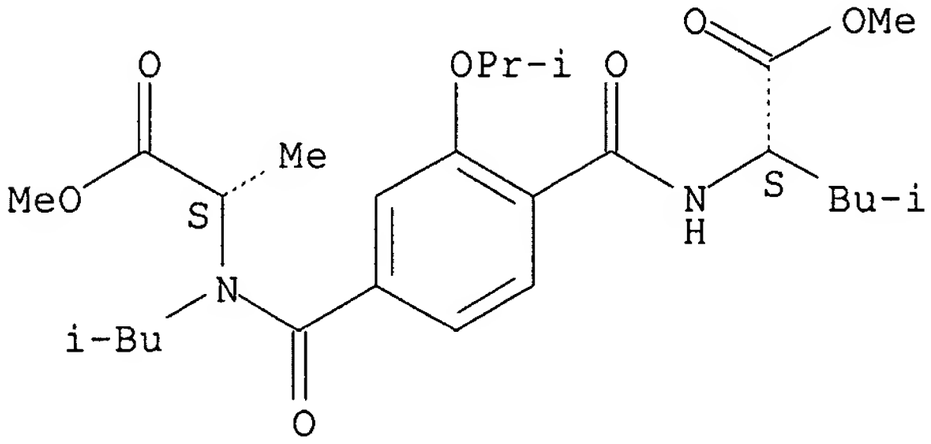
100.0% PROCESSED    79581 ITERATIONS                                35 ANSWERS
SEARCH TIME: 00.00.02

L2            35 SEA SSS FUL L1

=> d scan

L2    35 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN    L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-
      methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
      (9CI)
MF    C26 H40 N2 O7

Absolute stereochemistry.  Rotation (-).
```

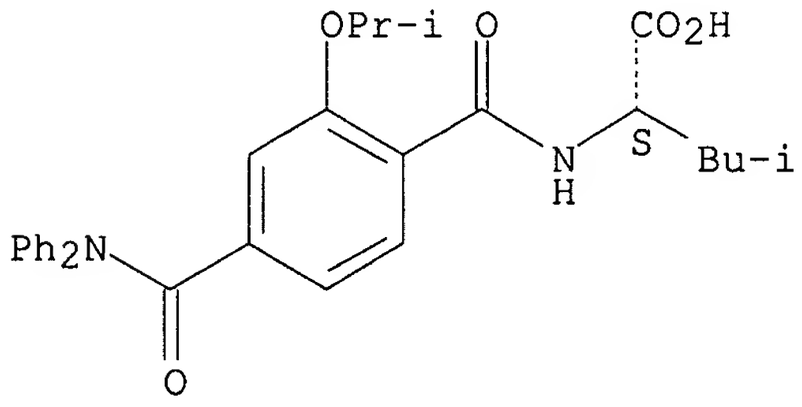



```
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):35

L2    35 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN    L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
MF    C29 H32 N2 O5

Absolute stereochemistry.  Rotation (-).
```

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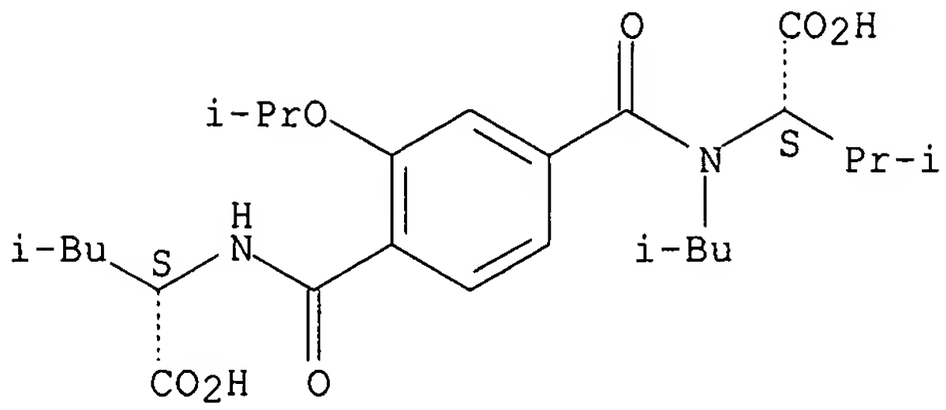
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**


L2    35 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN    L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-
      methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI)
MF    C26 H40 N2 O7
```

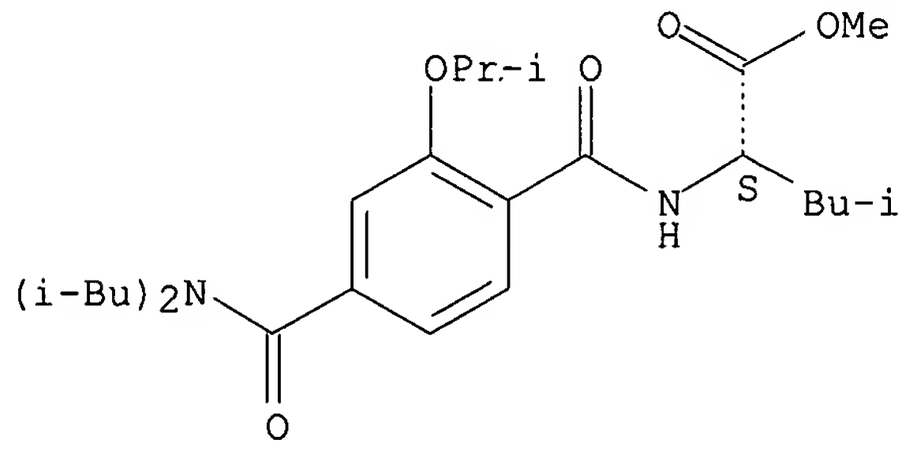
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C26 H42 N2 O5

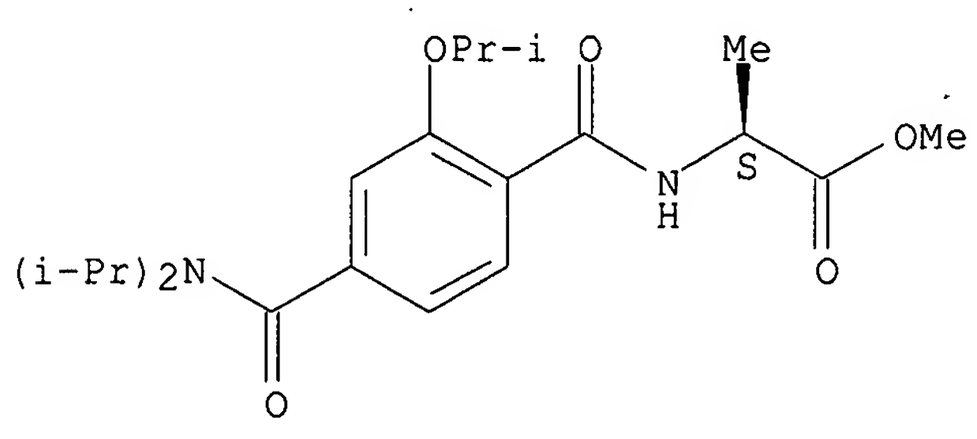
Absolute stereochemistry.  Rotation (+).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C21 H32 N2 O5

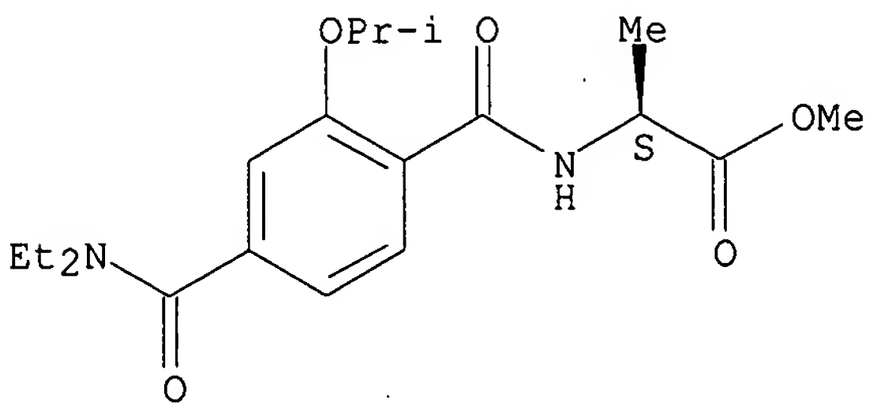
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C19 H28 N2 O5

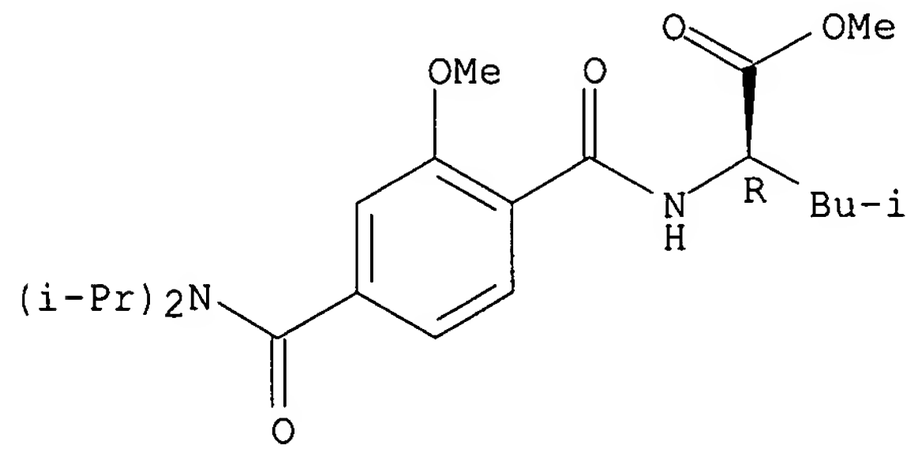
Absolute stereochemistry.  Rotation (+).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester
MF  C22 H34 N2 O5

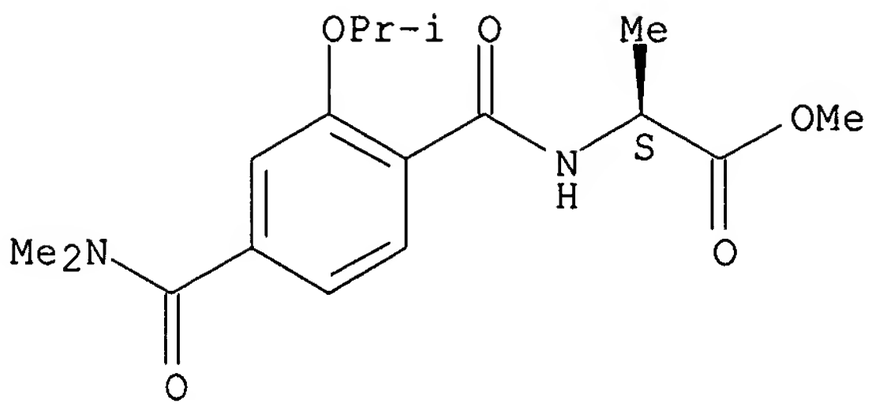
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C17 H24 N2 O5

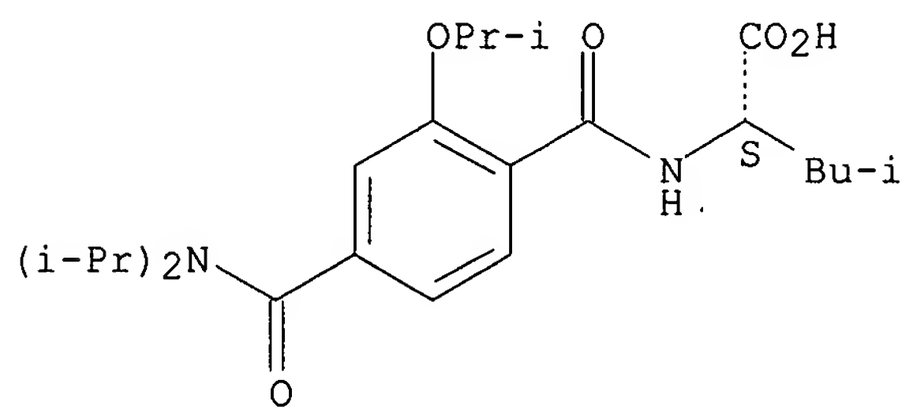
Absolute stereochemistry.  Rotation (+).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-
MF C23 H36 N2 O5

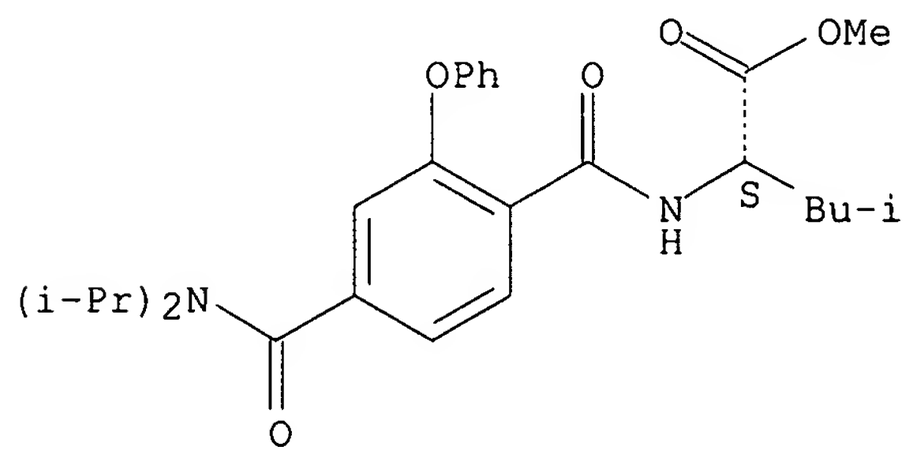
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-, methyl ester
MF C27 H36 N2 O5

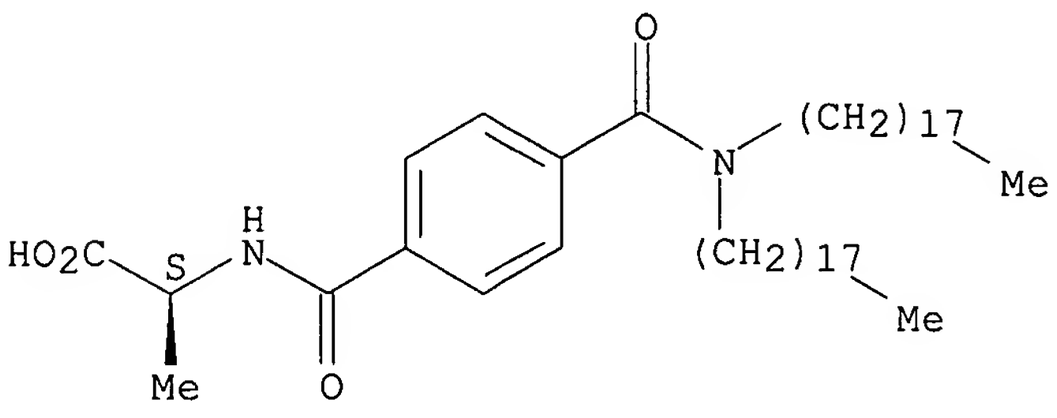
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]-
MF  C47 H84 N2 O4

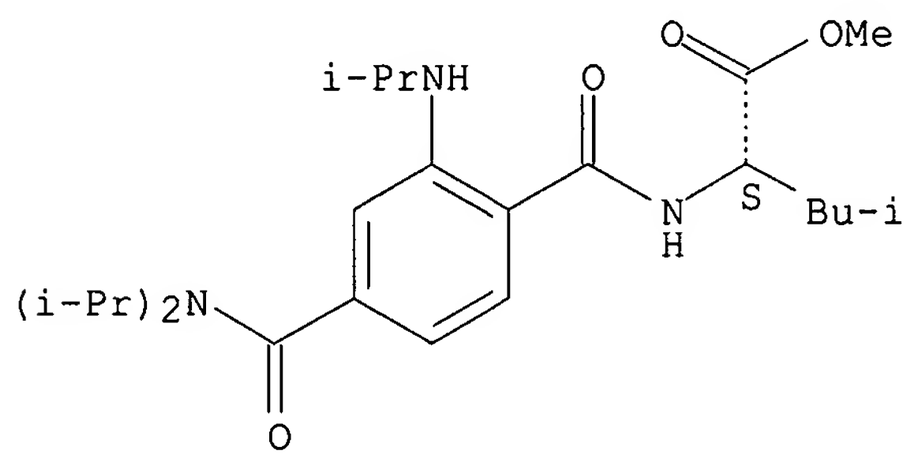
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]-, methyl ester
MF  C24 H39 N3 O4

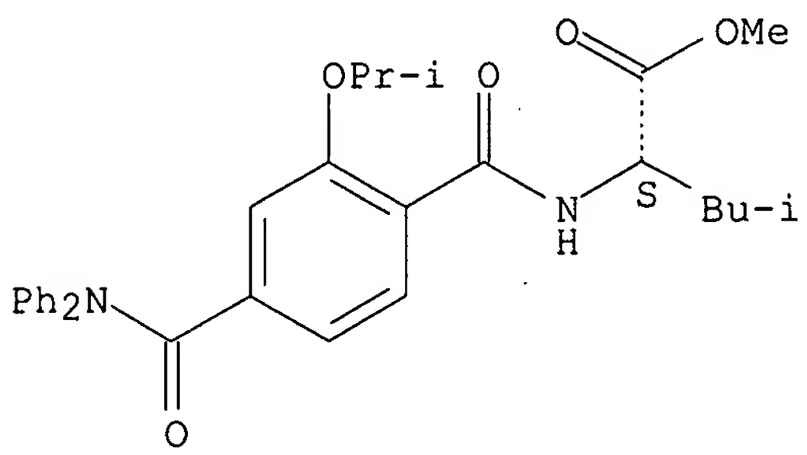
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

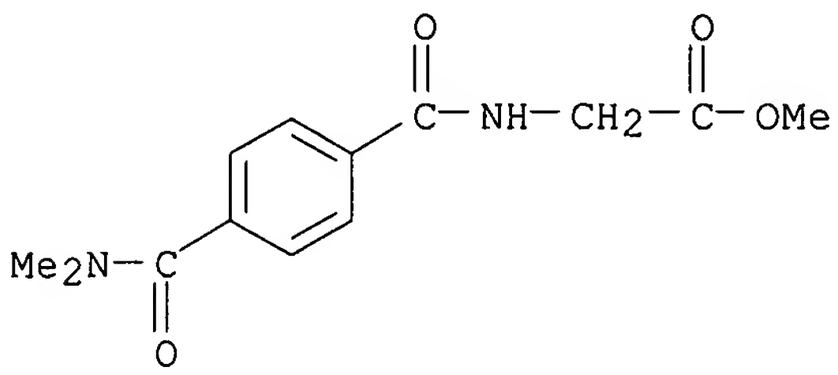
L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C30 H34 N2 O5

Absolute stereochemistry.  Rotation (-).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

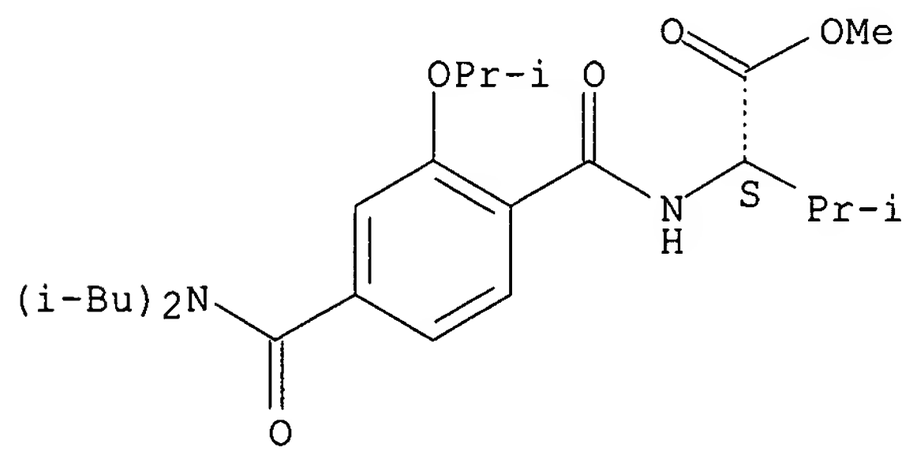
L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  Glycine, N-[4-[(dimethylamino)carbonyl]benzoyl]-, methyl ester
MF  C13 H16 N2 O4



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C25 H40 N2 O5

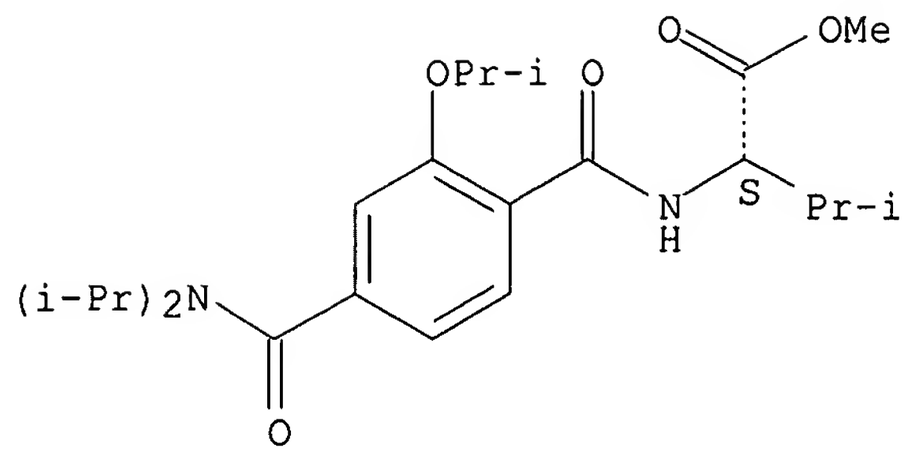
Absolute stereochemistry.  Rotation (+).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C23 H36 N2 O5

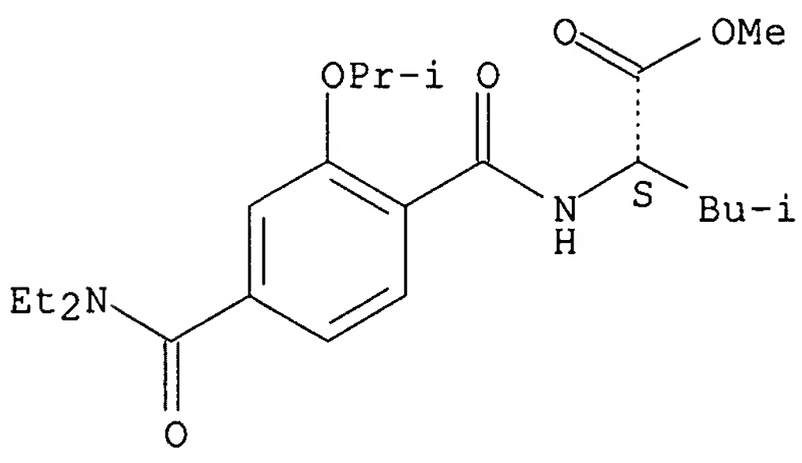
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C22 H34 N2 O5

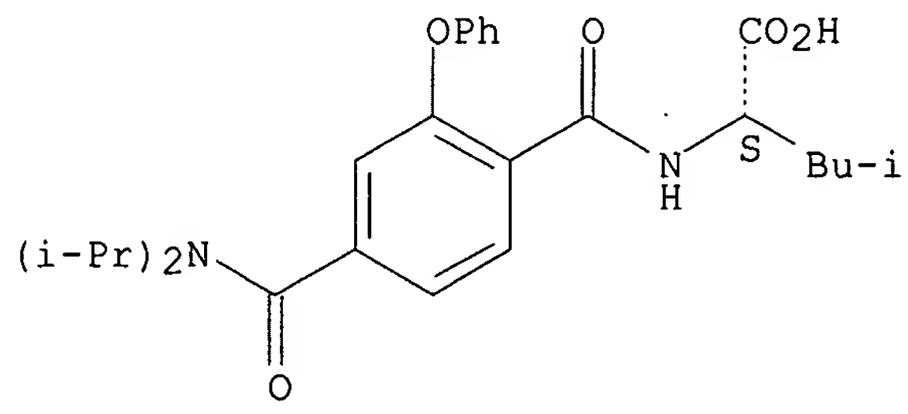
Absolute stereochemistry.  Rotation (+).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-
MF  C26 H34 N2 O5

Absolute stereochemistry.

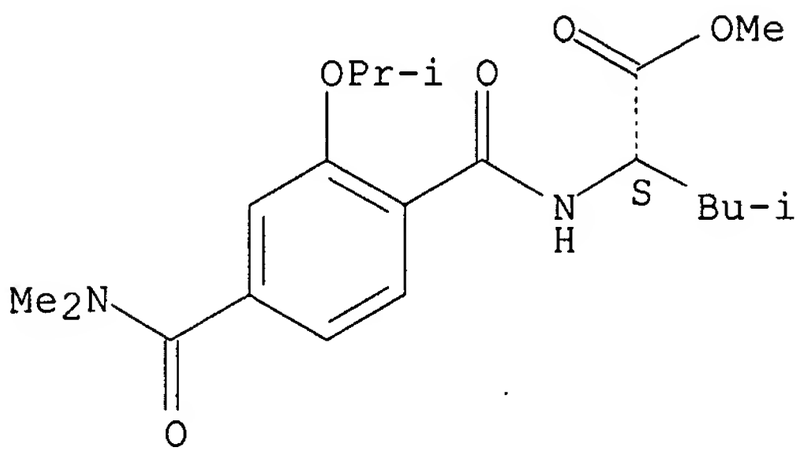


**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,

methyl ester
MF C20 H30 N2 O5

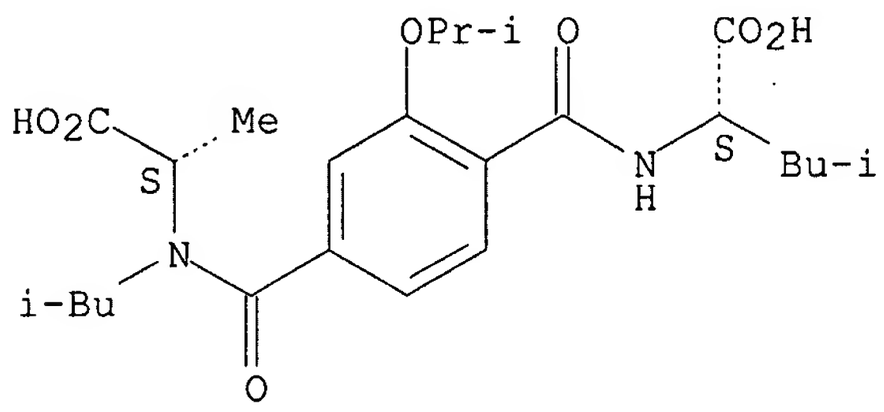
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI)
MF C24 H36 N2 O7

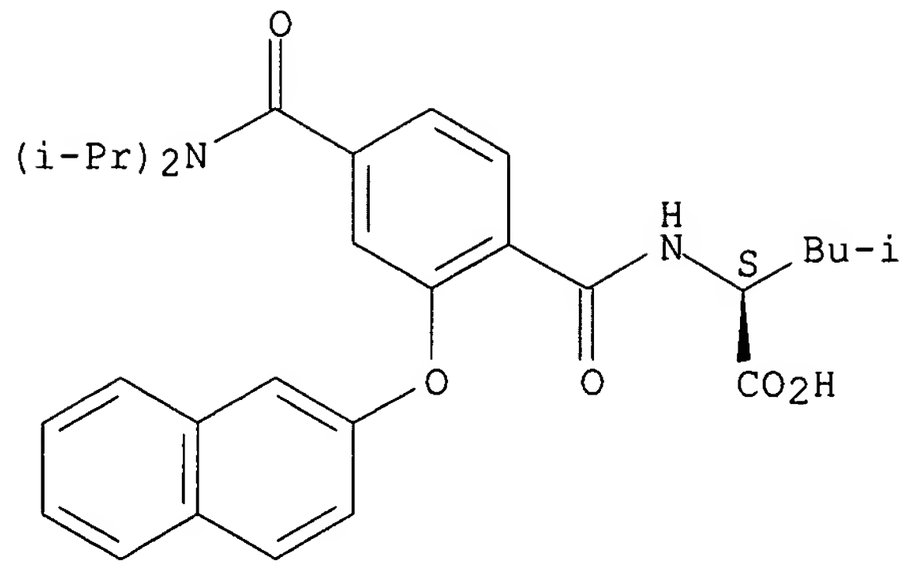
Absolute stereochemistry. Rotation (-).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(2-naphthalenyloxy)benzoyl]-
MF C30 H36 N2 O5

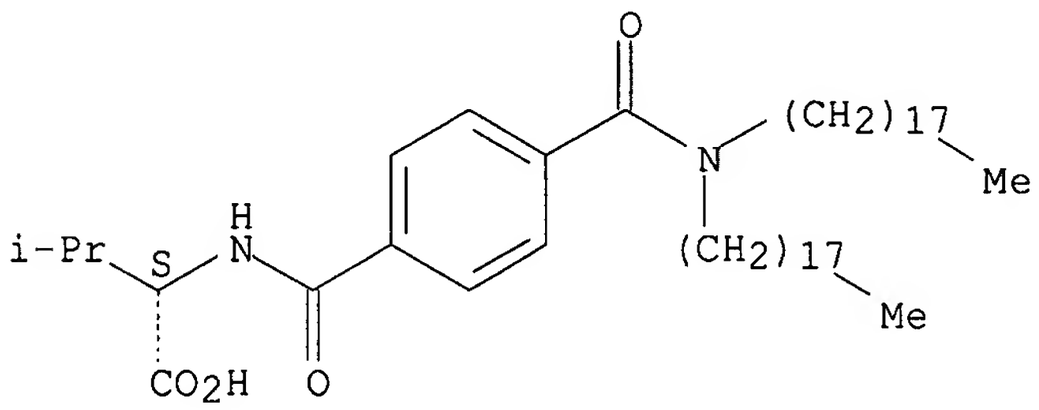
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Valine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]-
MF C49 H88 N2 O4

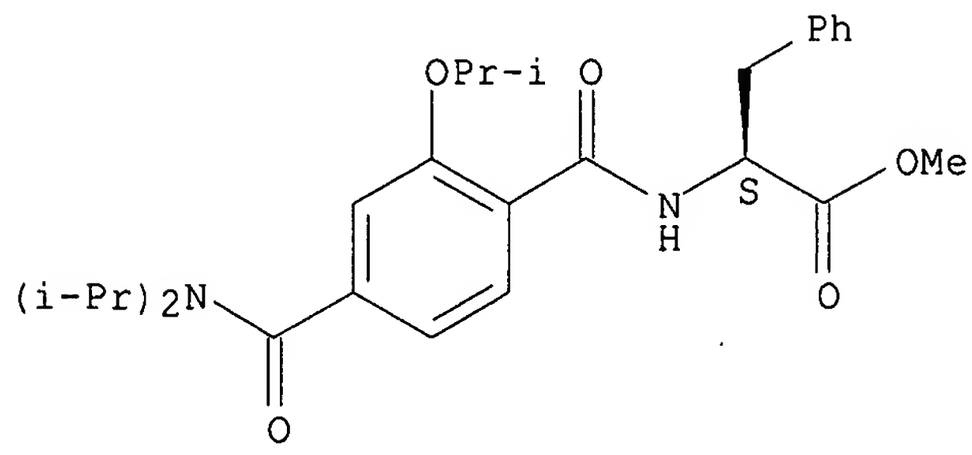
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF C27 H36 N2 O5

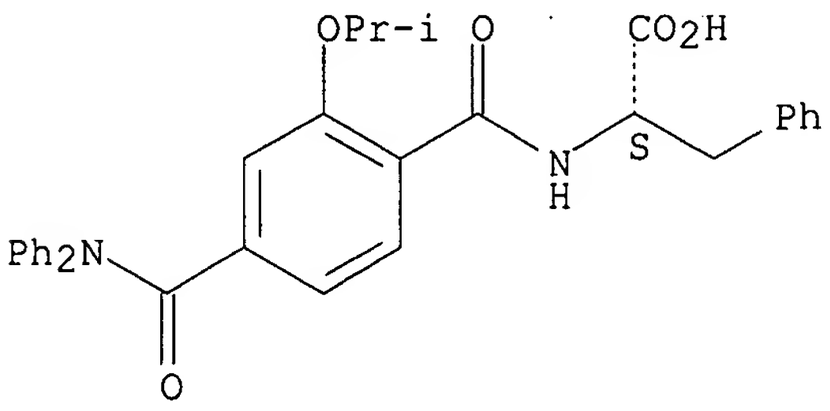
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
MF  C32 H30 N2 O5

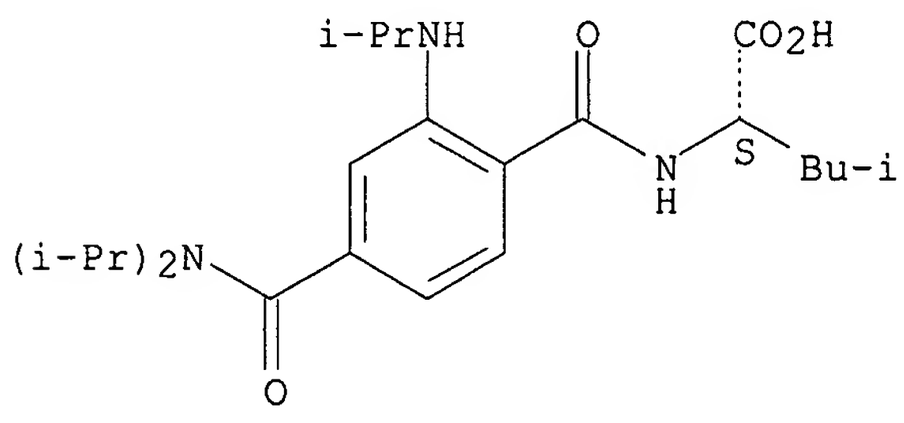
Absolute stereochemistry. Rotation (+).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]-
MF  C23 H37 N3 O4

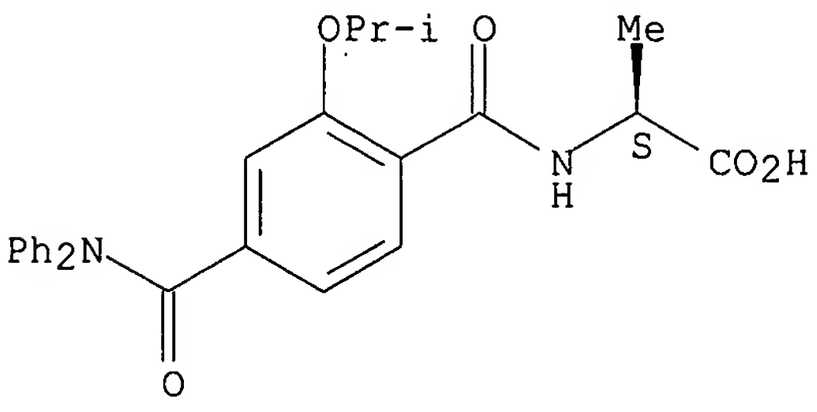
Absolute stereochemistry. Rotation (-).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
MF  C26 H26 N2 O5

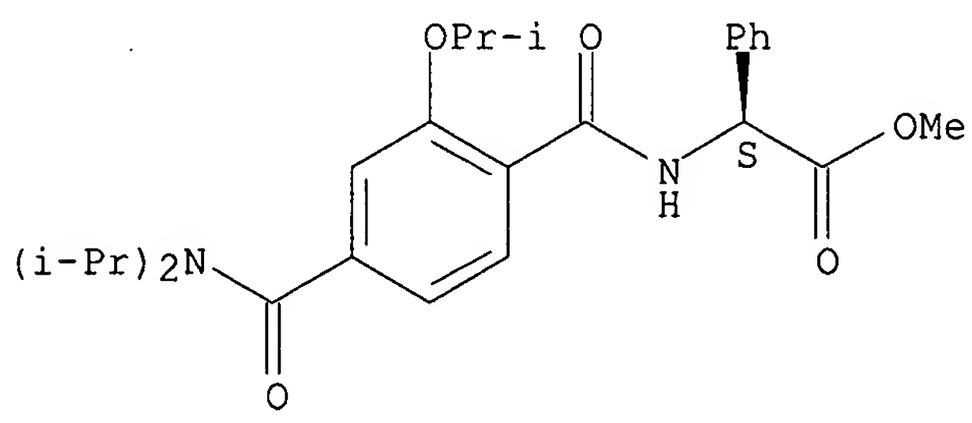
Absolute stereochemistry. Rotation (+).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  Benzeneacetic acid, α-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]amino]-, methyl ester, (αS)-
MF  C26 H34 N2 O5

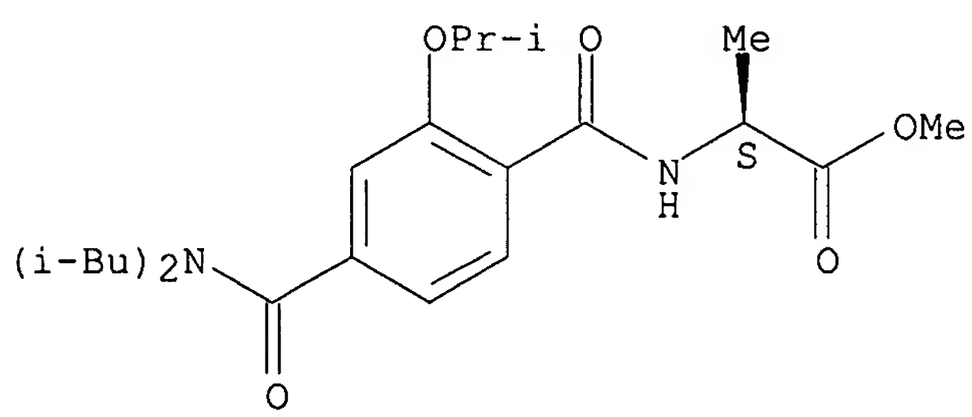
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C23 H36 N2 O5

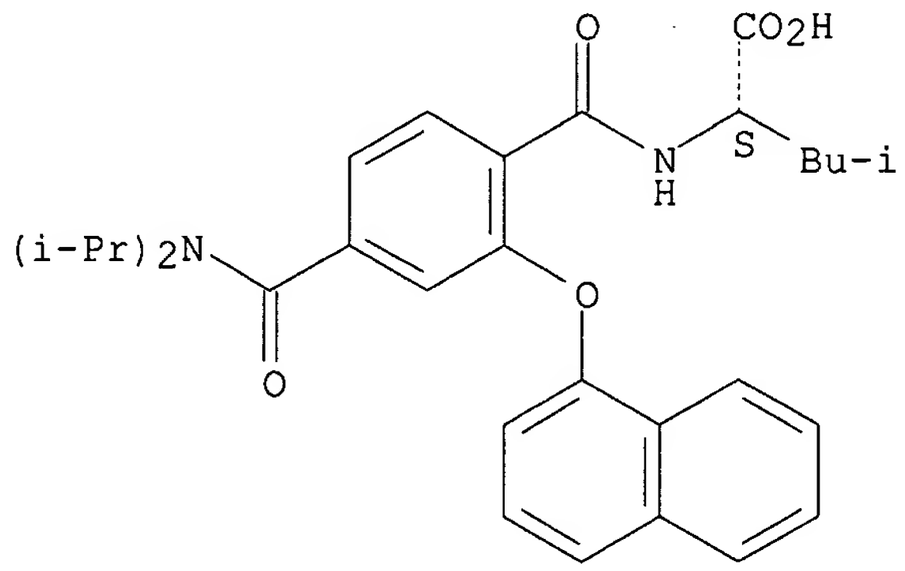
Absolute stereochemistry.  Rotation (+).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-naphthalenyloxy)benzoyl]-
MF  C30 H36 N2 O5

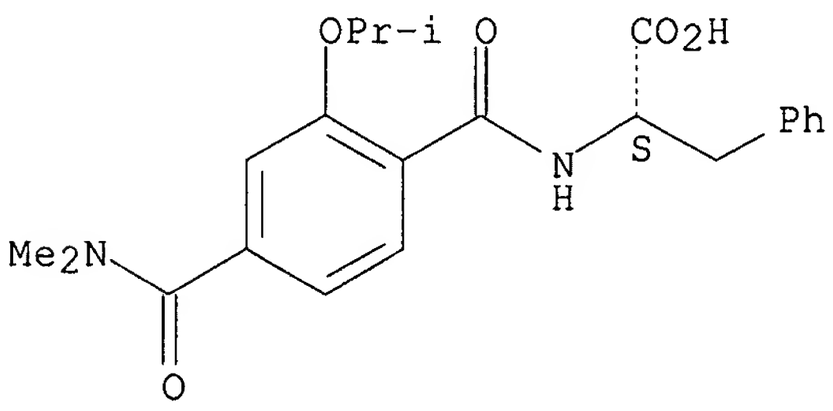
Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
MF C22 H26 N2 O5

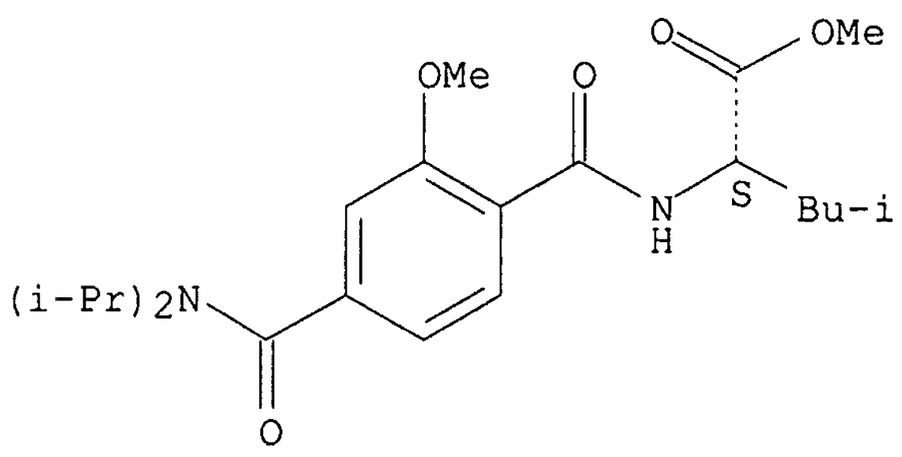
Absolute stereochemistry. Rotation (+).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2 35 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester
MF C22 H34 N2 O5

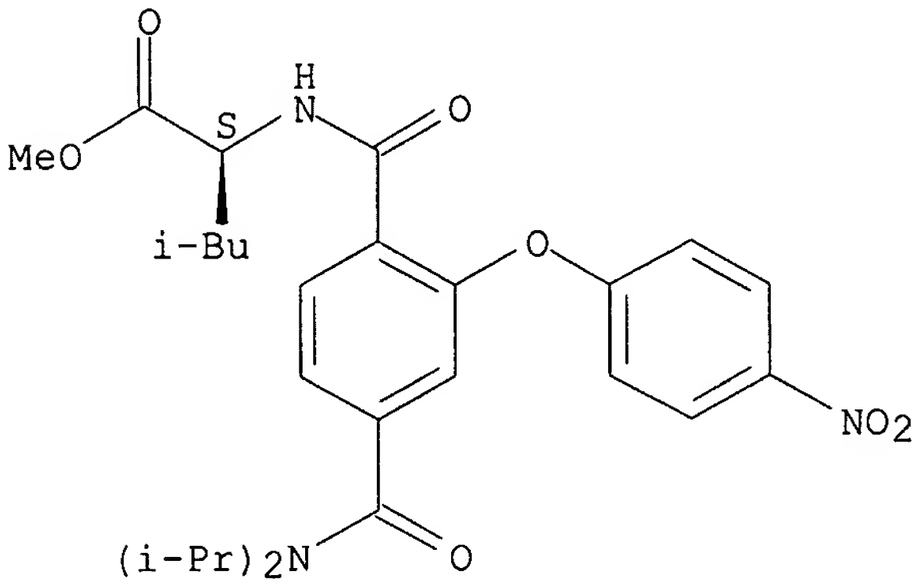
Absolute stereochemistry. Rotation (-).



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(4-nitrophenoxy)benzoyl]-, methyl ester
MF  C27 H35 N3 O7

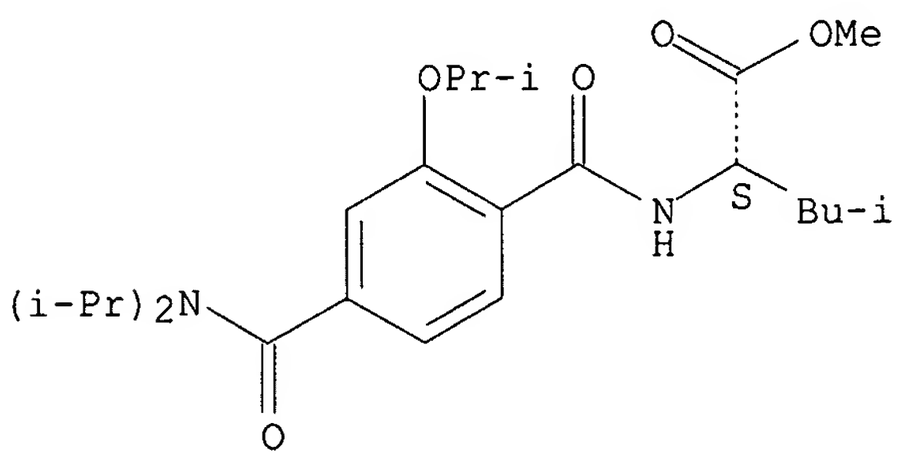
Absolute stereochemistry.




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester
MF  C24 H38 N2 O5

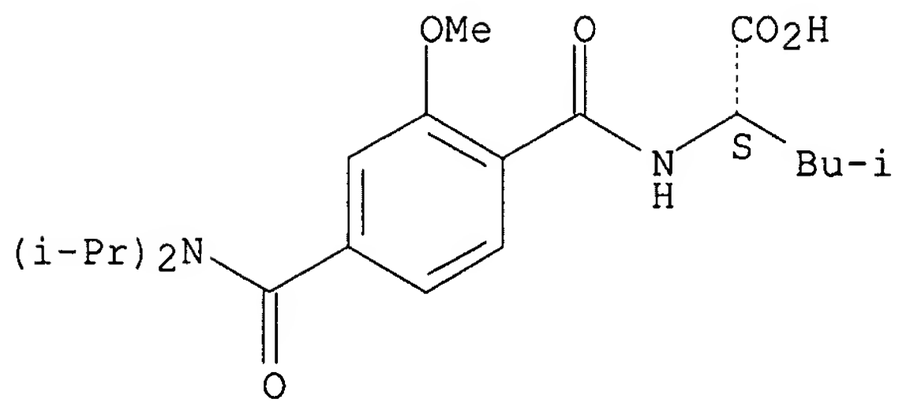
Absolute stereochemistry.  Rotation (-).




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

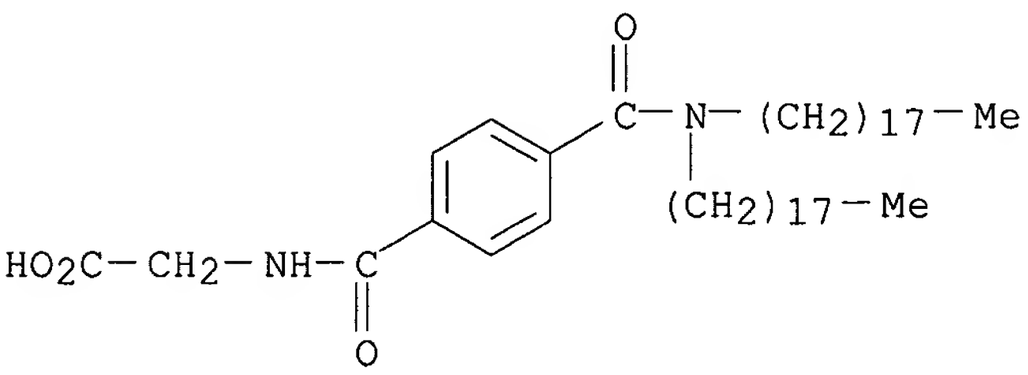
L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-
MF  C21 H32 N2 O5

Absolute stereochemistry.



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L2  35 ANSWERS  REGISTRY  COPYRIGHT 2008 ACS on STN
IN  Glycine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]-
MF  C46 H82 N2 O4



**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

ALL ANSWERS HAVE BEEN SCANNED

=> file caplus

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 179.28 | 179.49 |

FILE 'CAPLUS' ENTERED AT 14:34:02 ON 25 JAN 2008
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FILE COVERS 1907 - 25 Jan 2008  VOL 148 ISS 5
FILE LAST UPDATED: 24 Jan 2008  (20080124/ED)

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http://www.cas.org/infopolicy.html

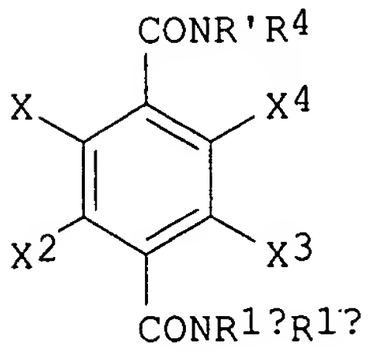
=> s l2
L3 5 L2

=> d l3 1-5 bib abs hitstr

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:961964 CAPLUS
DN 143:248664
TI Preparation of terephthalamide peptidomimetic compounds for therapeutic use
IN Hamilton, Andrew D.; Yin, Hang
PA Yale University, USA
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|---|
| PI | WO 2005079541 | A2 | 20050901 | WO 2005-US5557 | 20050222 |
| | WO 2005079541 | A3 | 20051103 | | |
| | W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| | RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| | AU 2005215051 | A1 | 20050901 | AU 2005-215051 | 20050222 |
| | CA 2556447 | A1 | 20050901 | CA 2005-2556447 | 20050222 |
| | EP 1723100 | A2 | 20061122 | EP 2005-713917 | 20050222 |
| | R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU | | | | |
| | US 2007123592 | A1 | 20070531 | US 2006-588478 | 20061002 |
| PRAI | US 2004-546111P | P | 20040219 | | |
| | WO 2005-US5557 | W | 20050222 | | |

OS CASREACT 143:248664; MARPAT 143:248664
GI

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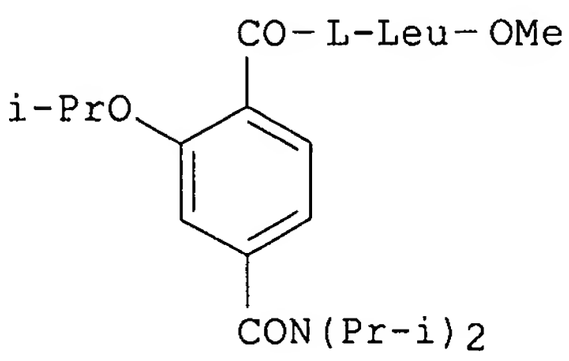



II

AB The invention relates to compds. and pharmaceutical compns. based on terephthalamide which are proteomimetic and methods for inhibiting the interaction of an α-helical protein with another protein or binding site and for treating diseases or conditions which are modulated through

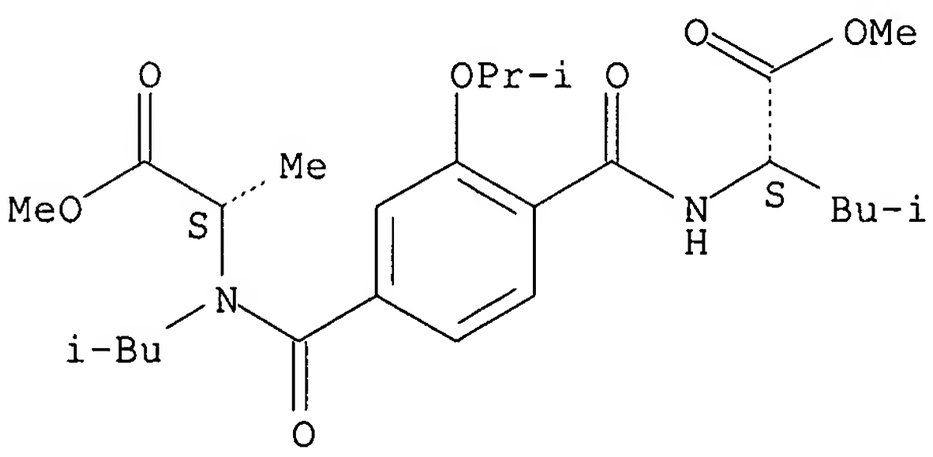
these interactions. Compds. I [X is H, halo, R, OR, SR or an amino group, where R is H, (un)substituted alkyl, acyl, aryl, heteroaryl, alkylenearyl or alkyleneheteroaryl; X2, X3, X4 are independently H, halo, OH, Rc, ORc, where Rc is (un)substituted alkyl, acyl, aryl or alkylenearyl; R4 is H, (un)substituted alkyl, alkenyl or alkylene amine; R', R1a, R1b are any group given for R4 or (CH2)0-2CHR2CO2H or an alkyl ester, where R2 is independently H or (un)substituted hydrocarbon, alkoxy, ester, alkanol, alkanoic acid, amine, etc.; or N-R' or NR1aR1b form an amino acid residue] are claimed. Thus, peptidomimetic compound II, prepared via coupling reaction of L-leucine Me ester hydrochloride, showed inhibitory constant Ki = 0.781 ± 0.070 μM in a fluorescence polarization assay (binding affinity for Bcl-XL).

IT 681466-00-2P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(conformation; preparation of terephthalamide peptidomimetic compds. for therapeutic use)

RN 681466-00-2 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

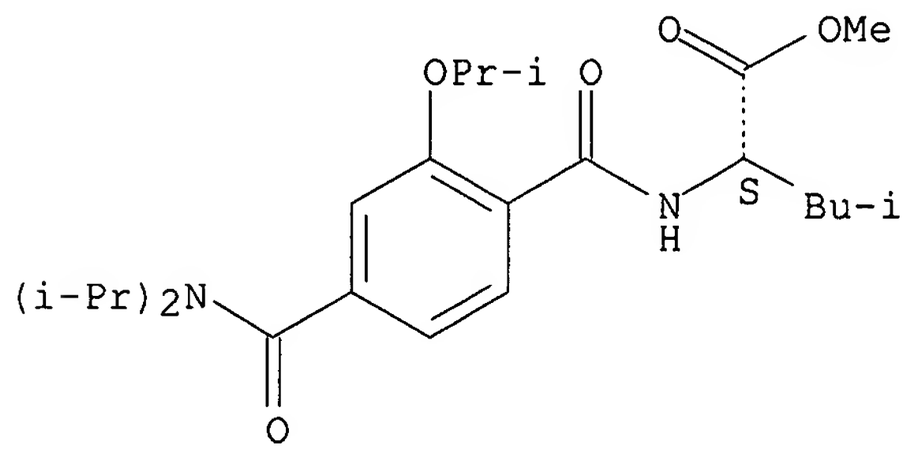



IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of terephthalamide peptidomimetic compds. for therapeutic use)

RN 681465-54-3 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

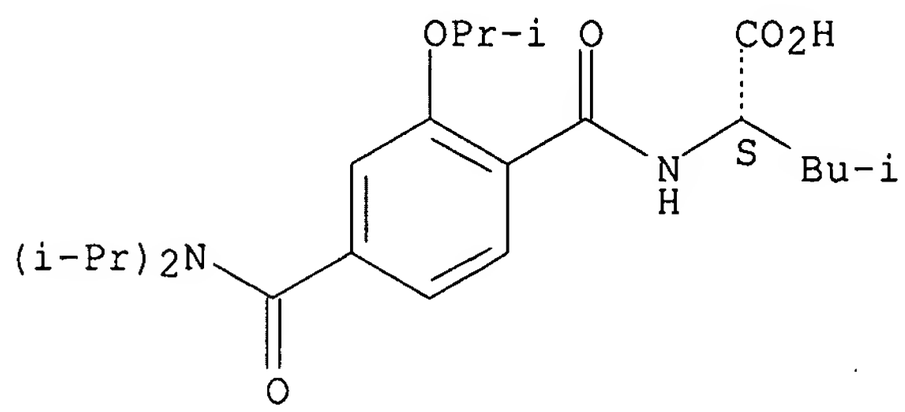



IT 681465-56-5P 681465-60-1P 681465-62-3P
681465-64-5P 681465-66-7P 681465-68-9P
681465-70-3P 681465-74-7P 681465-80-5P
681465-82-7P 852065-21-5P 852065-22-6P

852065-23-7P 852065-25-9P 852065-26-0P
852065-27-1P 852065-28-2P 852065-29-3P
852065-30-6P 852065-31-7P 852065-32-8P
852065-33-9P 852065-34-0P 852065-35-1P
852065-36-2P 852065-37-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of terephthalamide peptidomimetic compds. for therapeutic use)

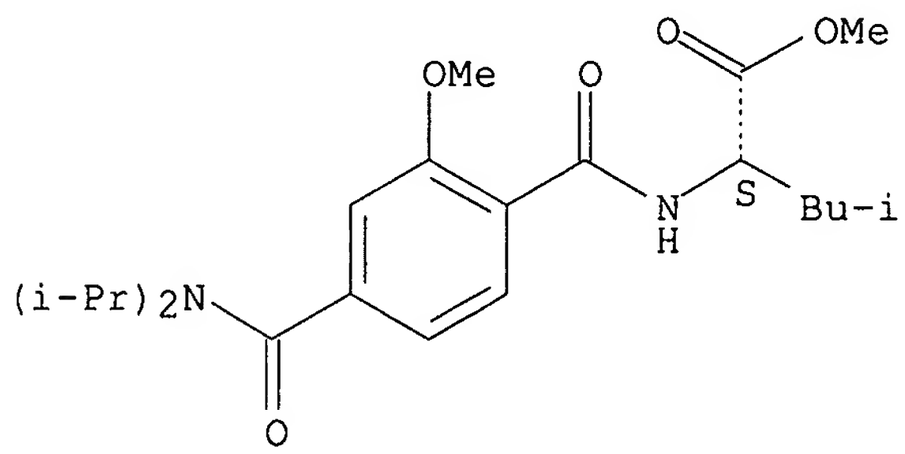
RN 681465-56-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



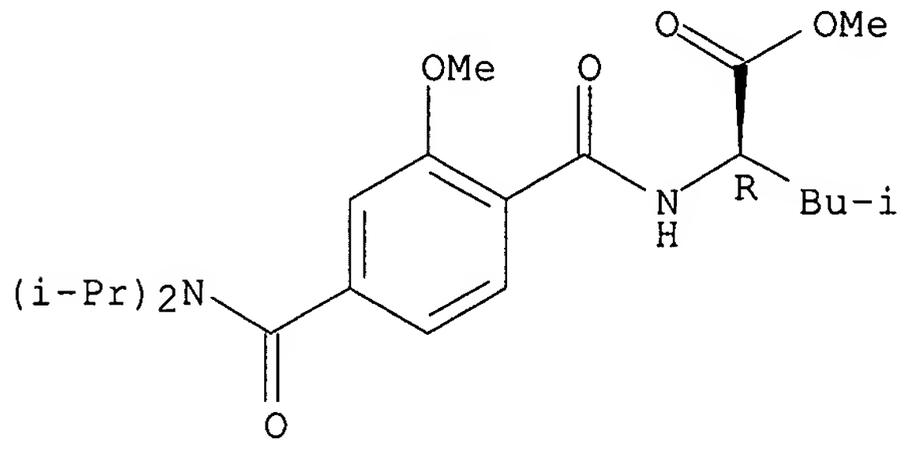

RN 681465-60-1 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).




RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

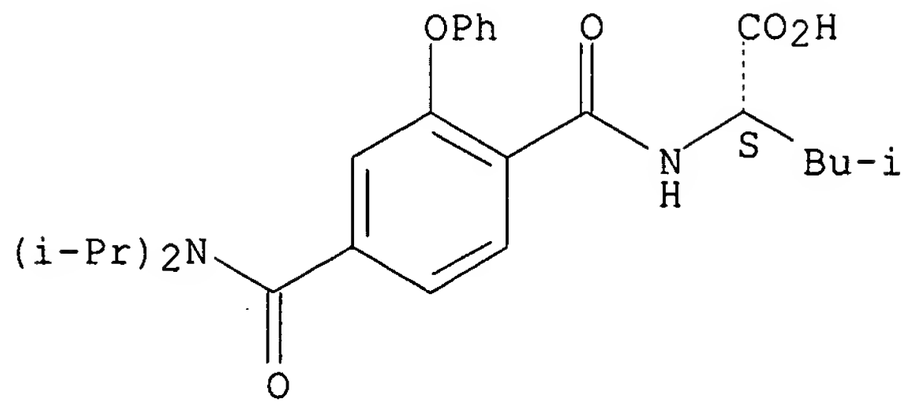
Absolute stereochemistry.




RN 681465-64-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-

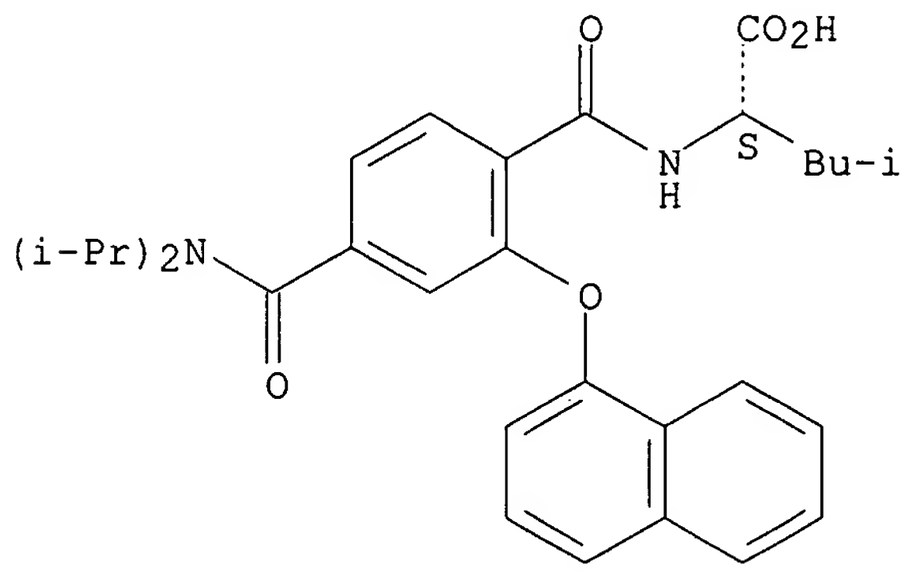
(CA INDEX NAME)

Absolute stereochemistry.



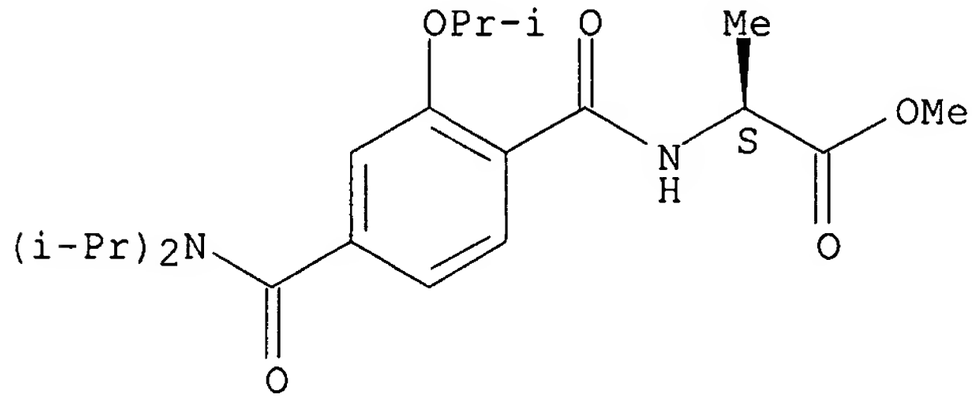

RN 681465-66-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-naphthalenyloxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



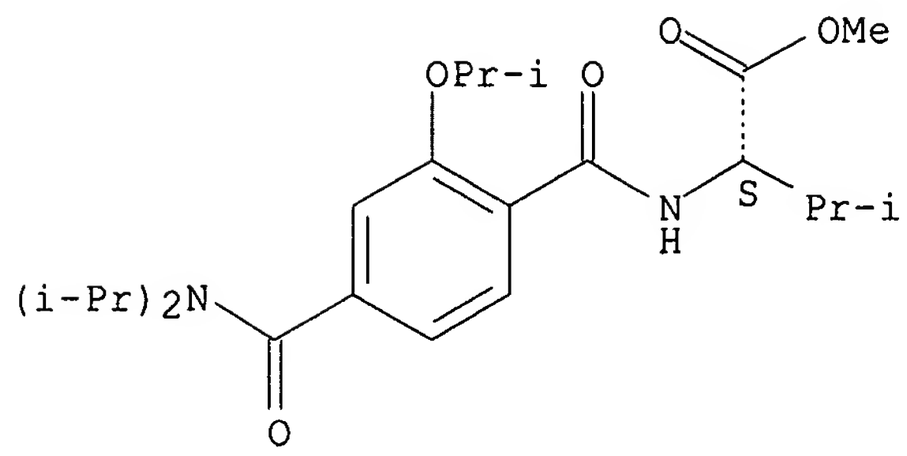

RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



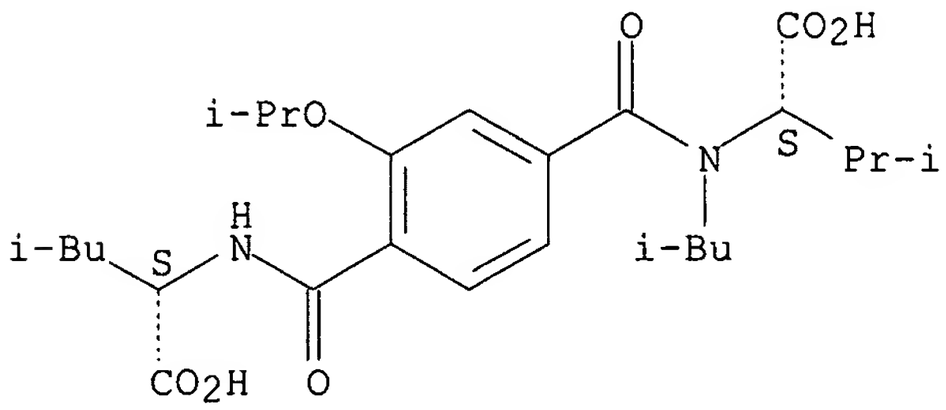

RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

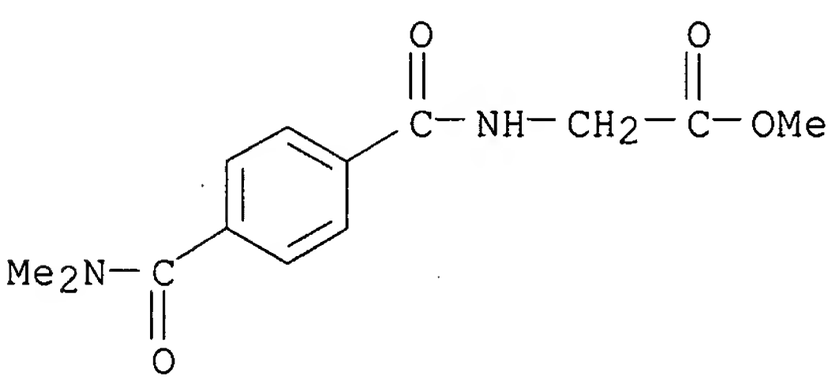


RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

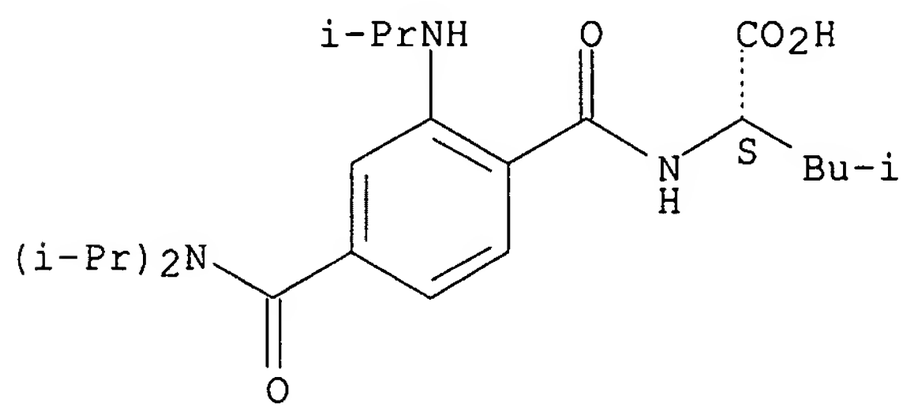


RN 681465-80-5 CAPLUS
CN Glycine, N-[4-[(dimethylamino)carbonyl]benzoyl]-, methyl ester (CA INDEX NAME)



RN 681465-82-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]- (CA INDEX NAME)

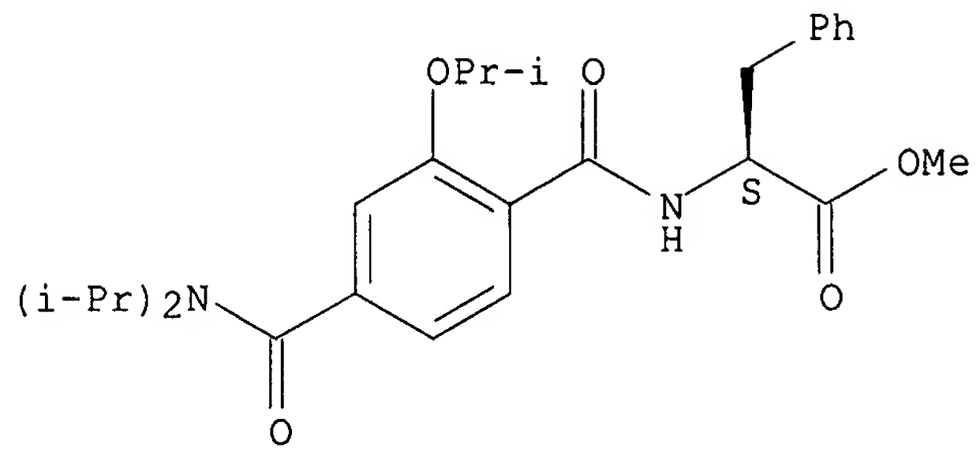
Absolute stereochemistry. Rotation (-).



RN 852065-21-5 CAPLUS
CN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-

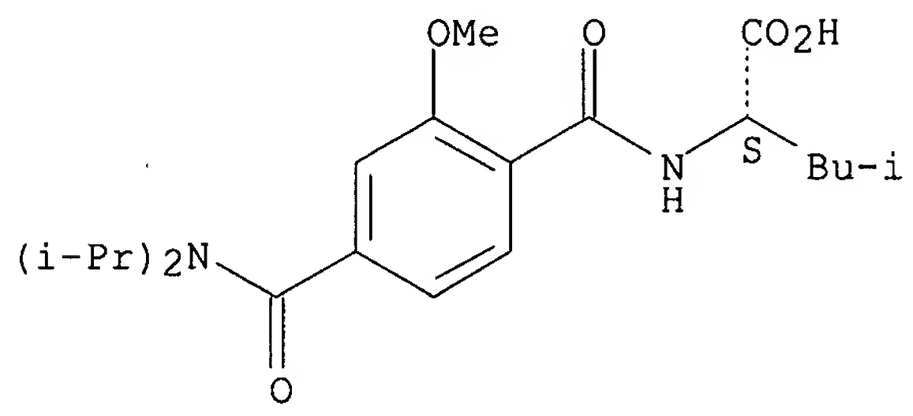
methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



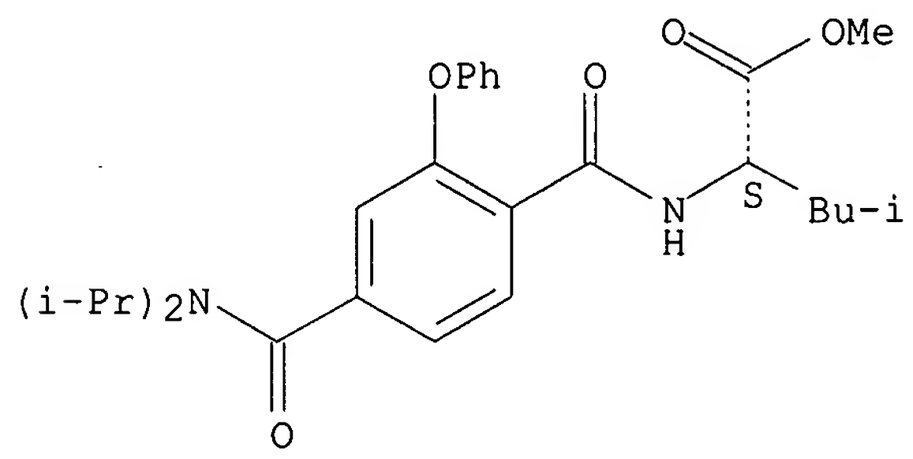

RN 852065-22-6 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-
(CA INDEX NAME)

Absolute stereochemistry.



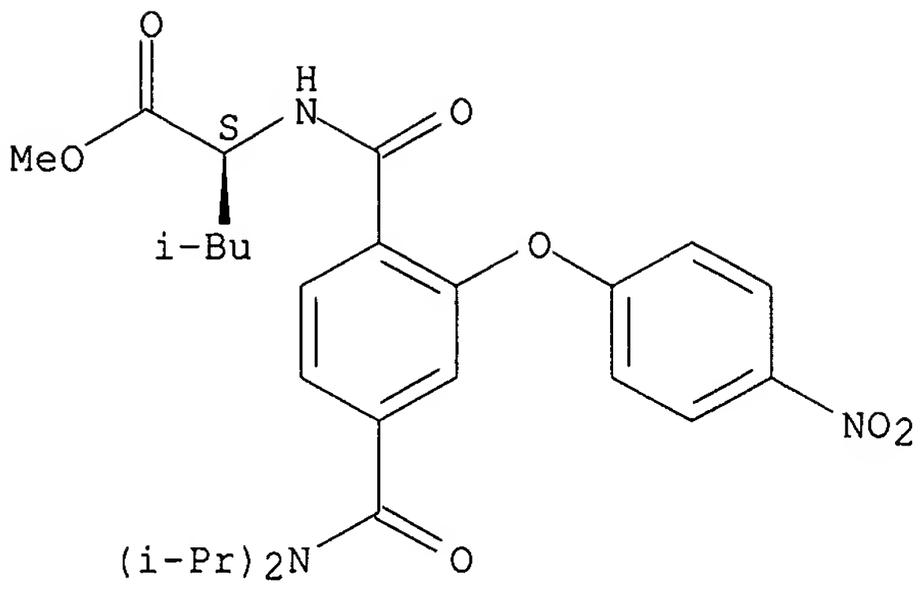

RN 852065-23-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry.



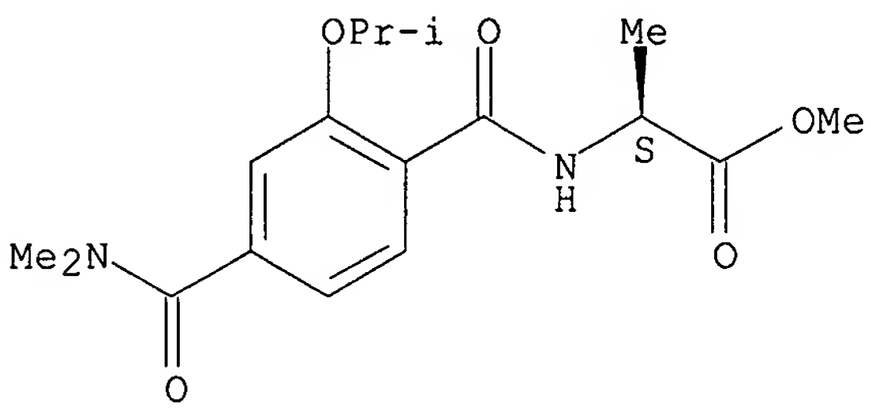

RN 852065-25-9 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(4-
nitrophenoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



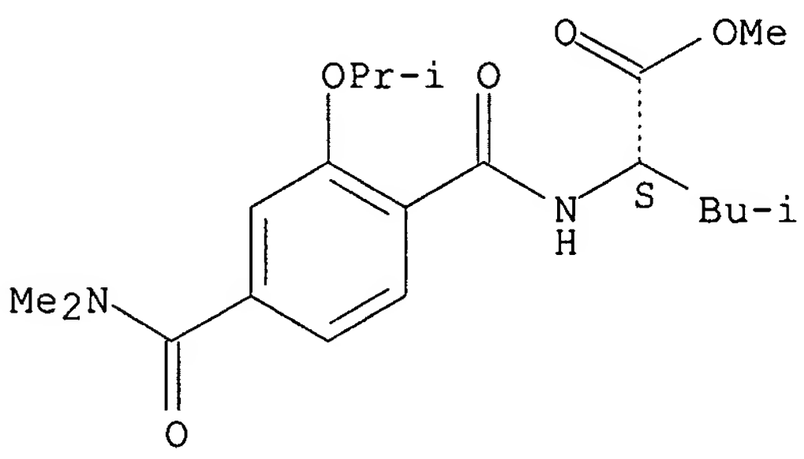
RN 852065-26-0 CAPLUS
CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



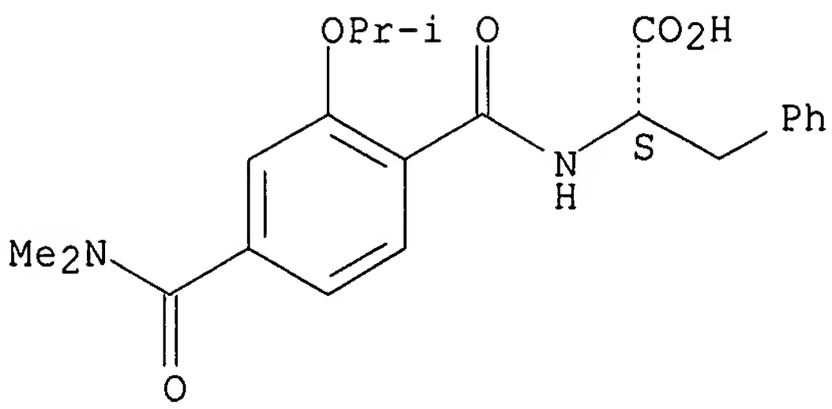
RN 852065-27-1 CAPLUS
CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



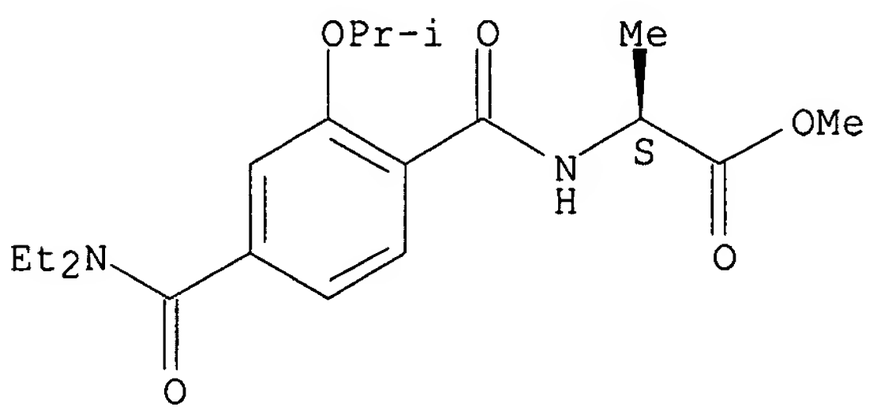
RN 852065-28-2 CAPLUS
CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



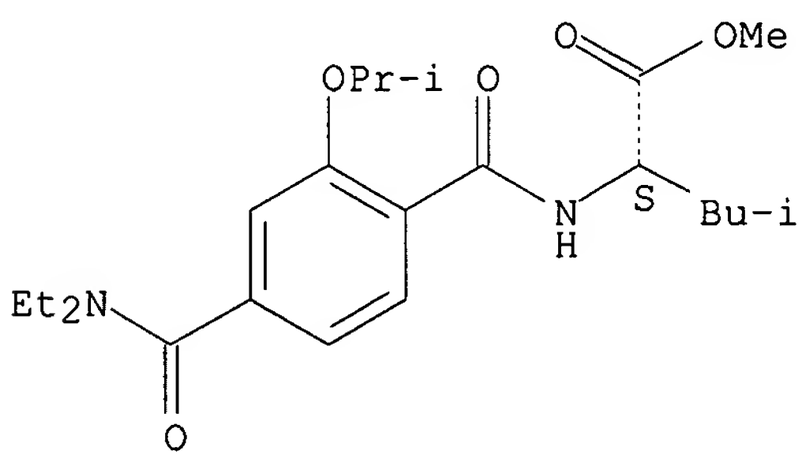
RN 852065-29-3 CAPLUS
CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



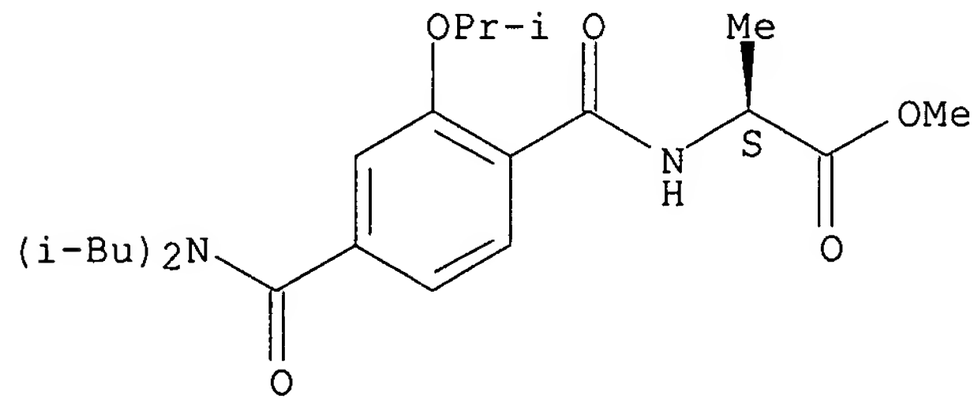
RN 852065-30-6 CAPLUS
CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 852065-31-7 CAPLUS
CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

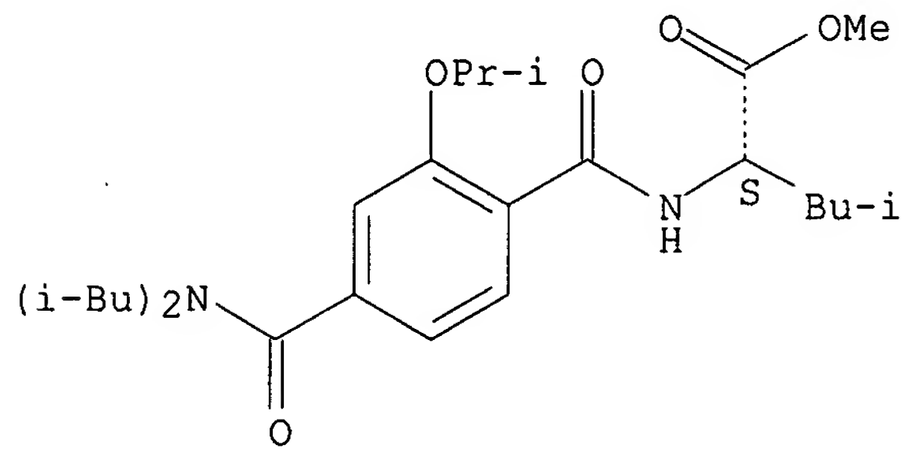
Absolute stereochemistry. Rotation (+).



RN 852065-32-8 CAPLUS

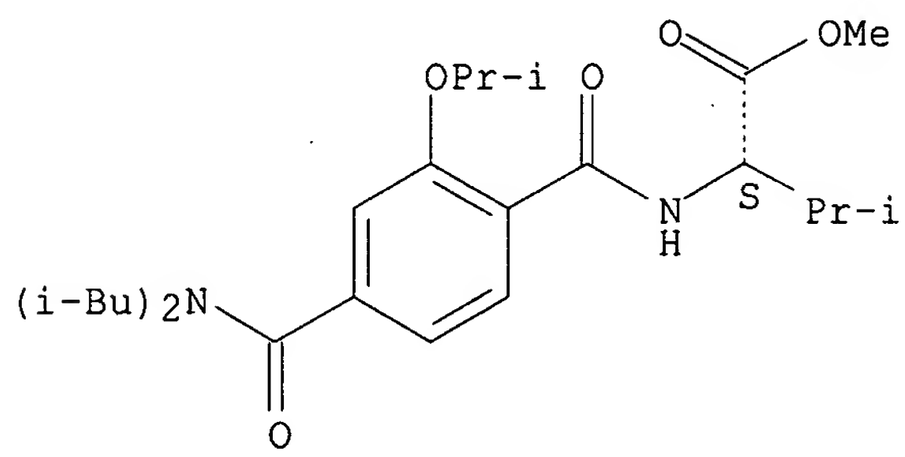
CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



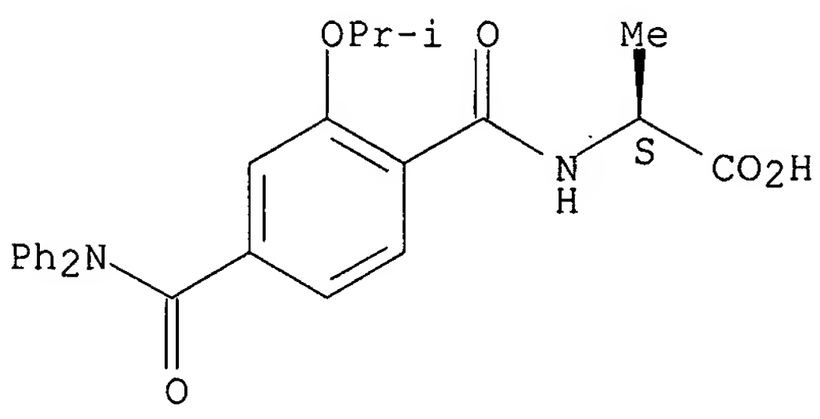

RN 852065-33-9 CAPLUS
CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



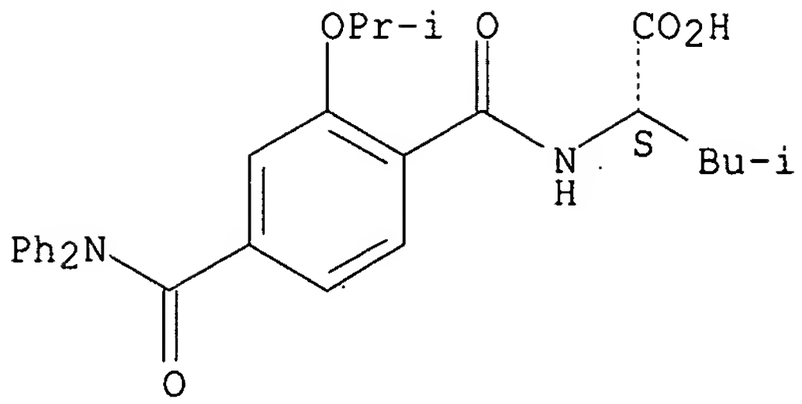

RN 852065-34-0 CAPLUS
CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



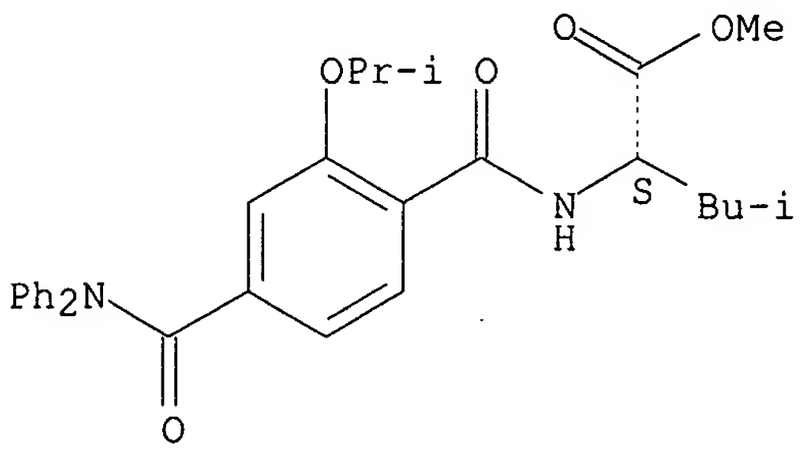

RN 852065-35-1 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



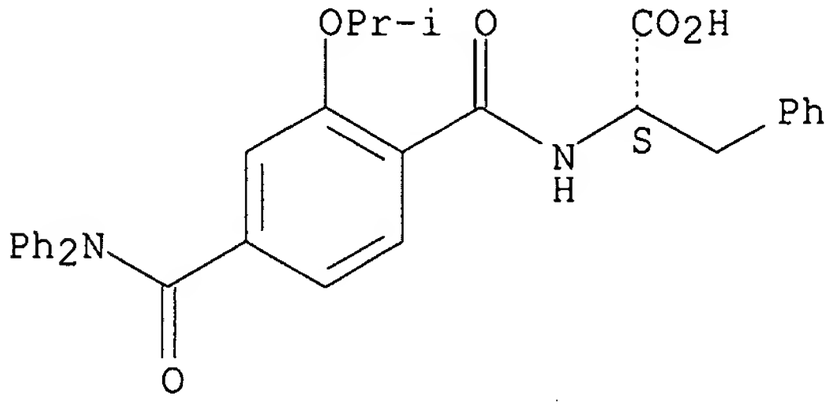
RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

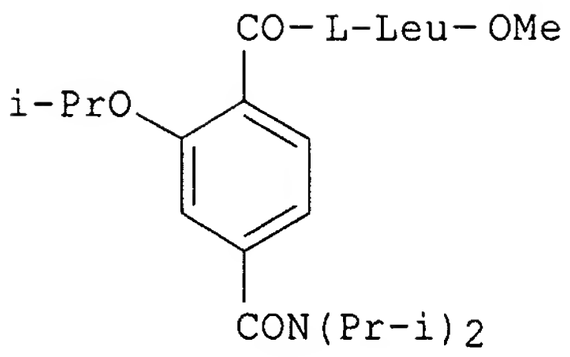


RN 852065-37-3 CAPLUS
CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

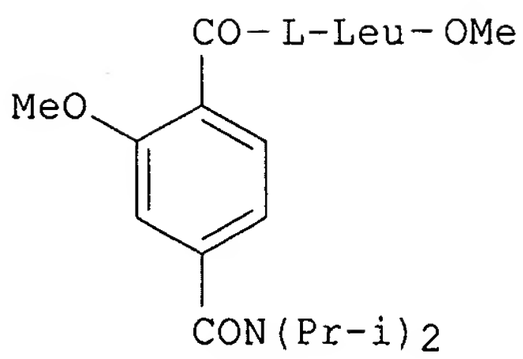
Absolute stereochemistry. Rotation (+).



L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
AN 2005:267006 CAPLUS
DN 142:482288
TI Terephthalamide Derivatives as Mimetics of Helical Peptides: Disruption of the Bcl-xL/Bak Interaction
AU Yin, Hang; Lee, Gui-in; Sedey, Kristine A.; Rodriguez, Johanna M.; Wang, Hong-Gang; Sebti, Said M.; Hamilton, Andrew D.
CS Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA
SO Journal of the American Chemical Society (2005), 127(15), 5463-5468
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 142:482288
GI




I




II

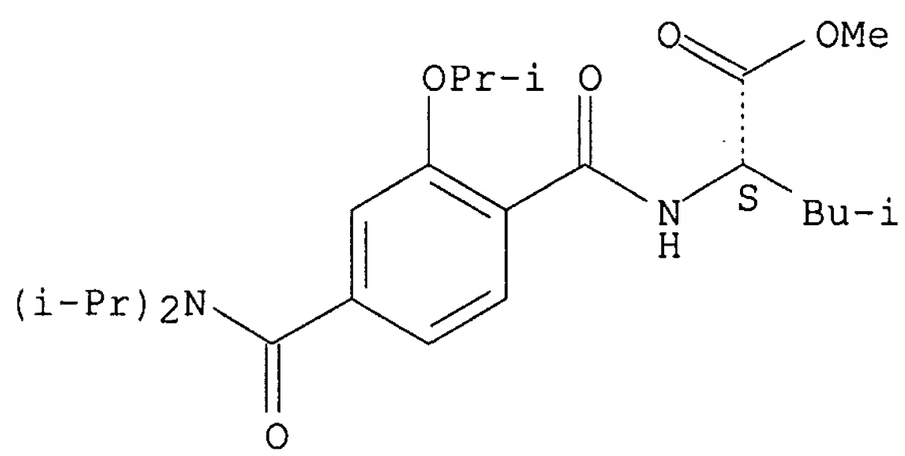
AB A series of Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, was designed to mimic the α-helical region of the Bak peptide. These mols. showed favorable in-vitro activities in disrupting the Bcl-xL/Bak BH3 domain complex (terephthalamides I and II, Ki = 0.78 ± 0.07 and 1.85 ± 0.32 μM, resp.). Extensive structure-affinity studies demonstrated a correlation between the ability of terephthalamide derivs. to disrupt Bcl-xL/Bak complex formation and the size of variable side chains on these mols. Treatment of human HEK293 cells with the terephthalamide derivative 26 resulted in disruption of the Bcl-xL/Bax interaction in whole cells with an IC50 of 35.0 μM. Computational docking simulations and NMR expts. suggested that the binding cleft for the BH3 domain of the Bak peptide on the surface of Bcl-xL is the target area for these synthetic inhibitors.

IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-54-3 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

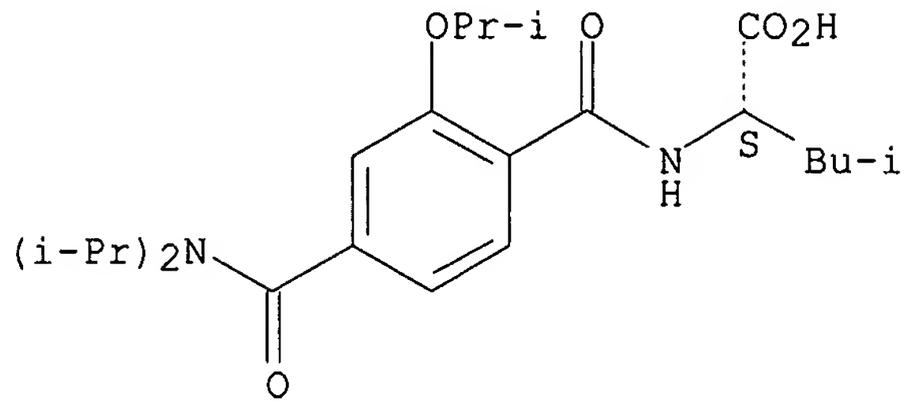



IT 681465-56-5P 681465-58-7P 681465-60-1P
681465-62-3P 681465-64-5P 681465-68-9P
681465-70-3P 681465-74-7P 681465-80-5P
681465-82-7P 852065-21-5P 852065-22-6P
852065-23-7P 852065-24-8P 852065-25-9P
852065-26-0P 852065-27-1P 852065-28-2P
852065-29-3P 852065-30-6P 852065-31-7P
852065-32-8P 852065-33-9P 852065-34-0P
852065-35-1P 852065-36-2P 852065-37-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-56-5 CAPLUS

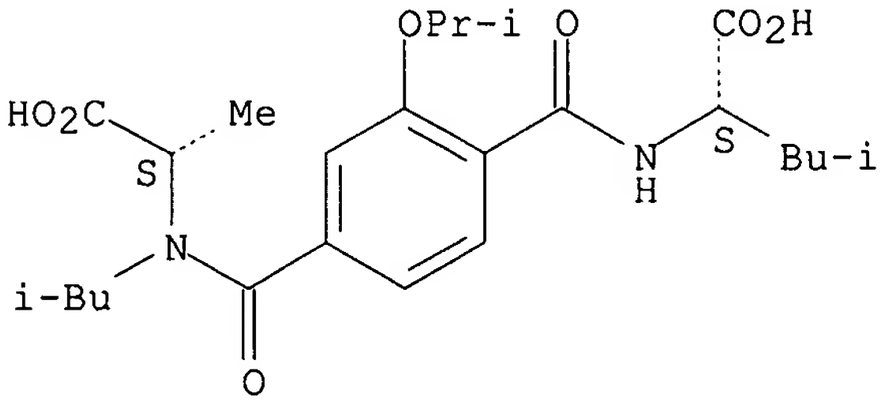
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



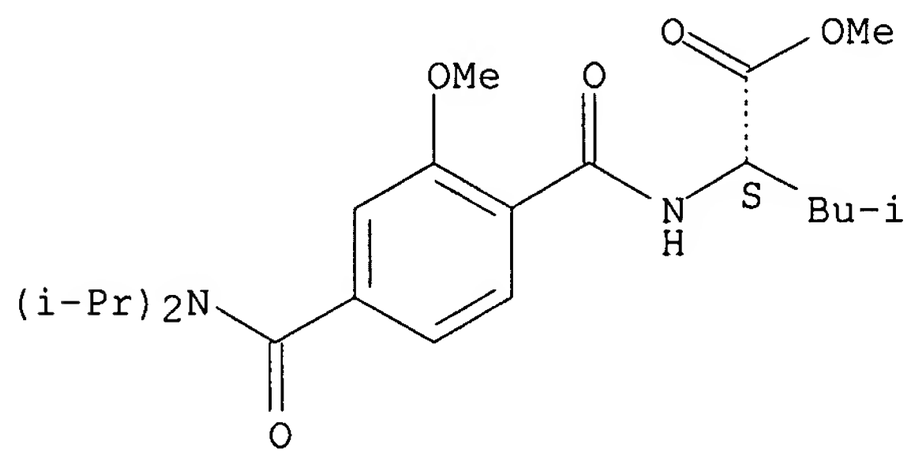
RN 681465-58-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



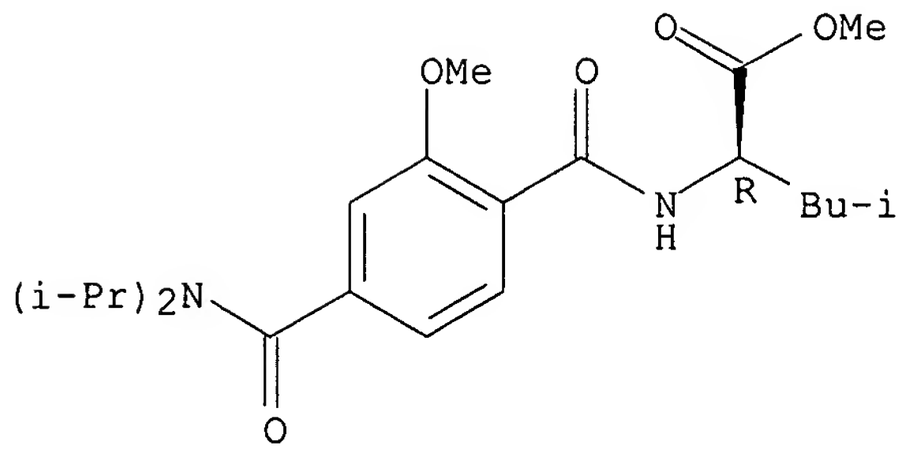
RN 681465-60-1 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



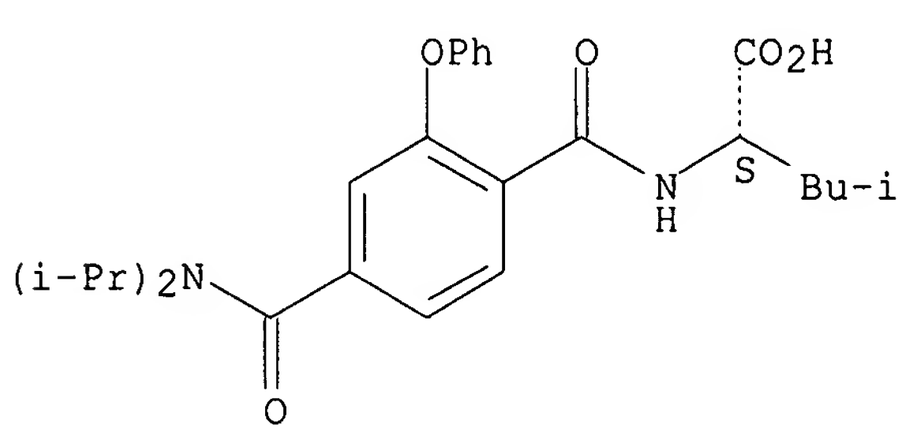
RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



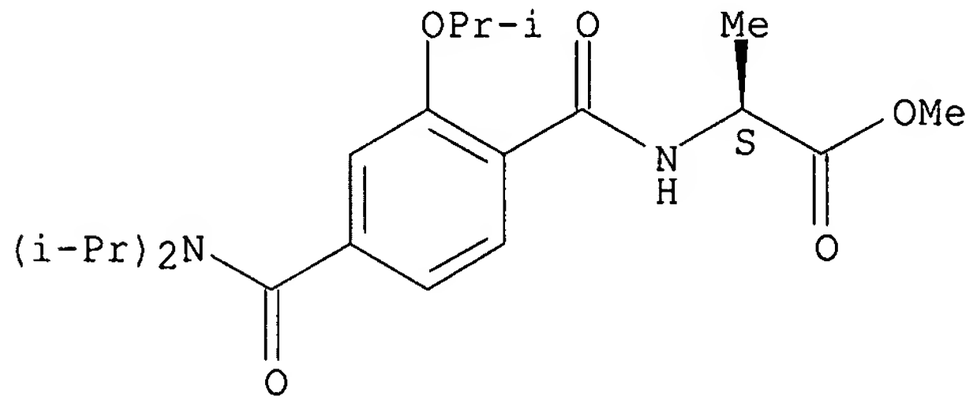
RN 681465-64-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-
(CA INDEX NAME)

Absolute stereochemistry.



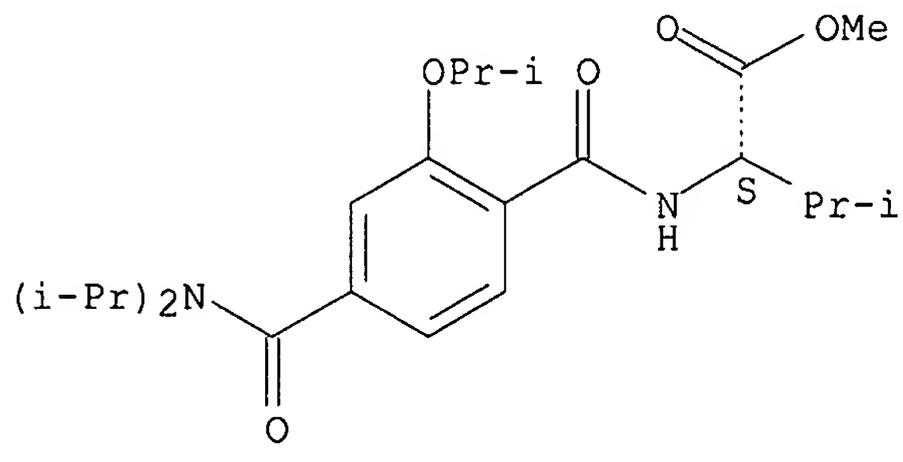
RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-
methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



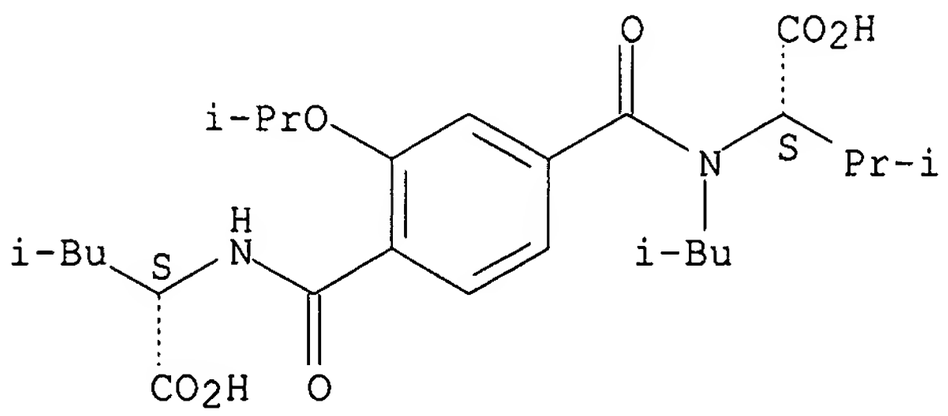
RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-
methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.

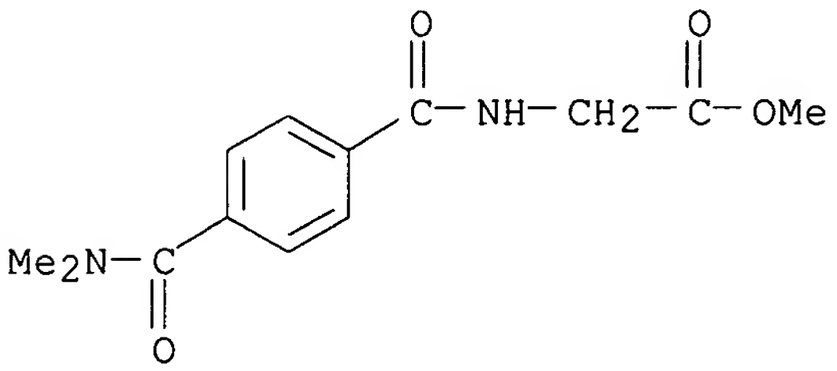


RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

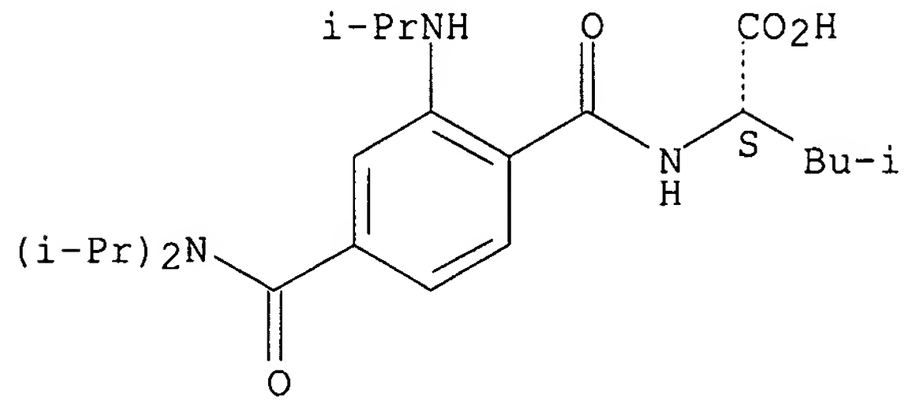


RN 681465-80-5 CAPLUS
CN Glycine, N-[4-[(dimethylamino)carbonyl]benzoyl]-, methyl ester (CA INDEX NAME)



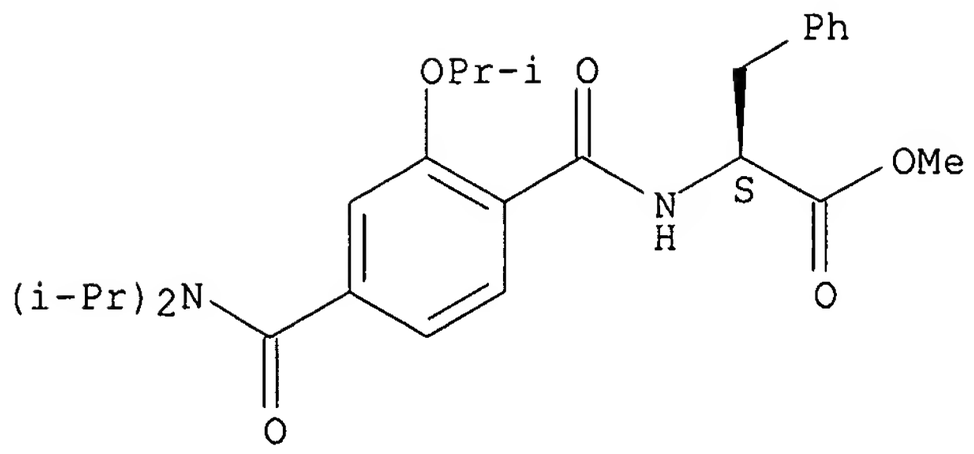
RN 681465-82-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



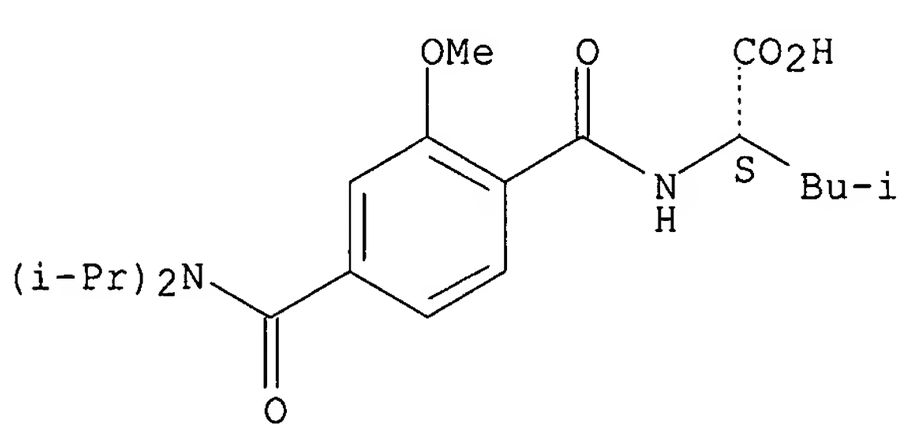
RN 852065-21-5 CAPLUS
CN L-Phenylalanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



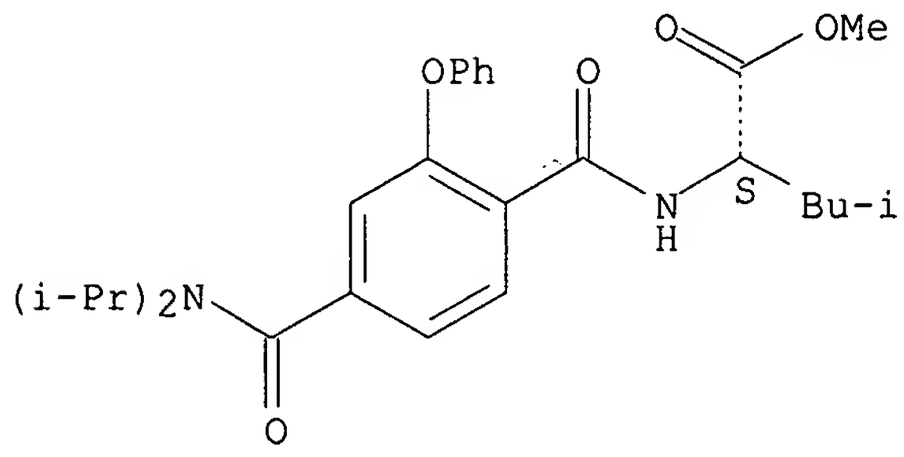
RN 852065-22-6 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-
(CA INDEX NAME)

Absolute stereochemistry.



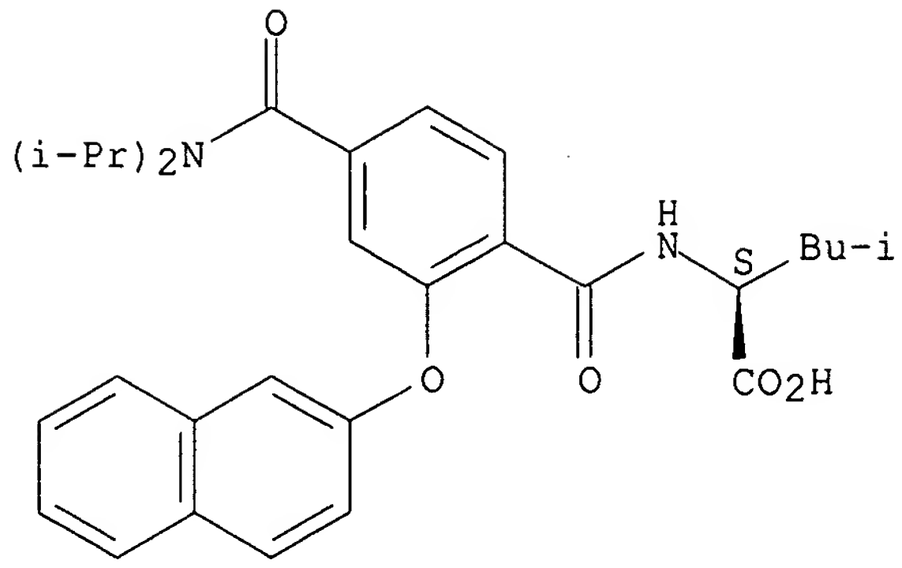
RN 852065-23-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry.



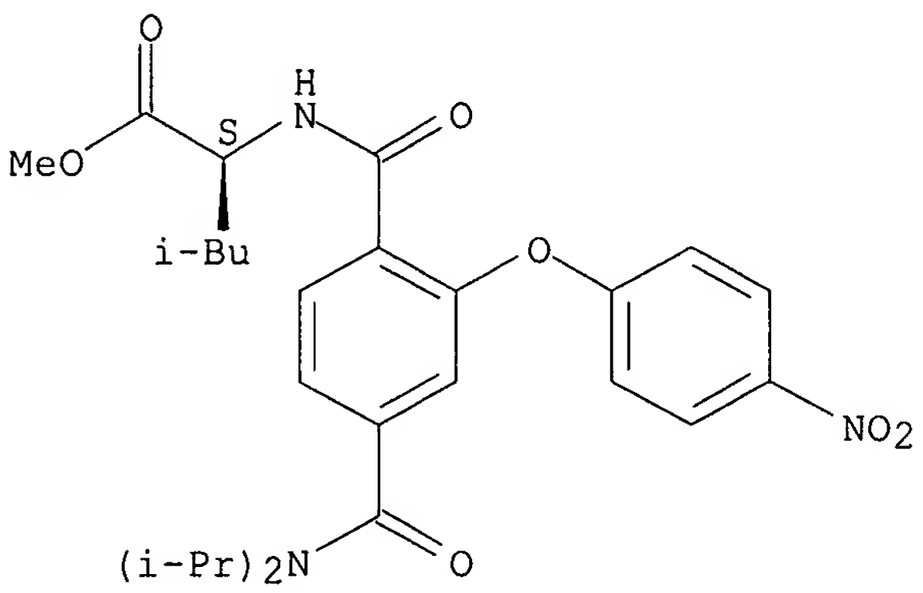
RN 852065-24-8 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(2-
naphthalenyloxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



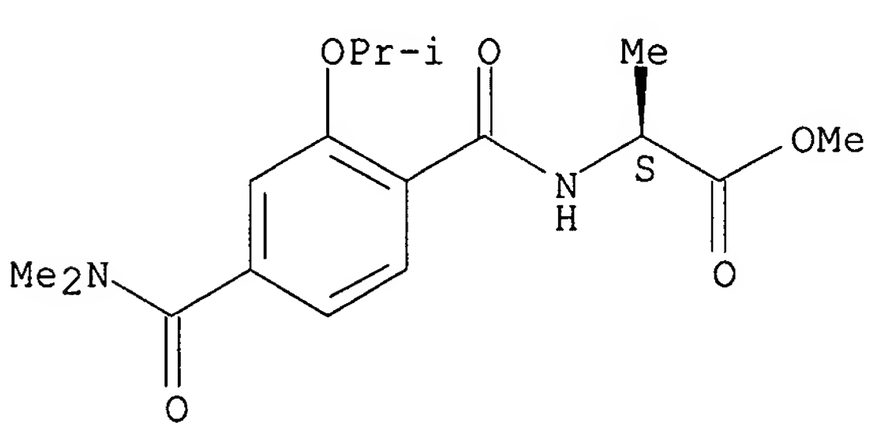
RN 852065-25-9 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(4-nitrophenoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



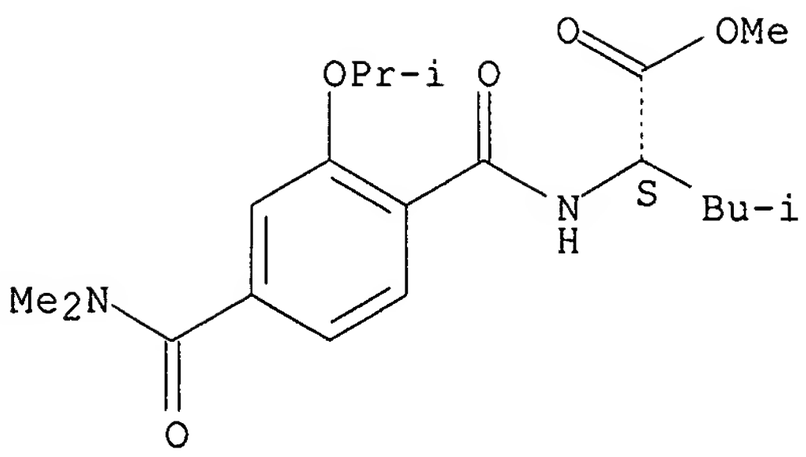
RN 852065-26-0 CAPLUS
CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



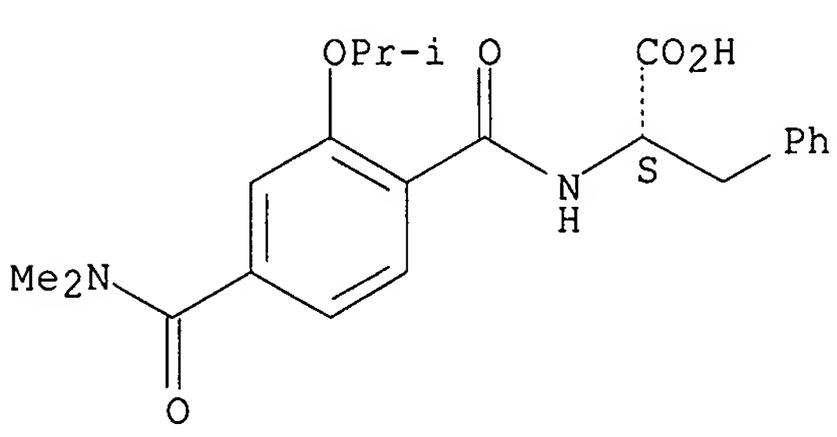
RN 852065-27-1 CAPLUS
CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



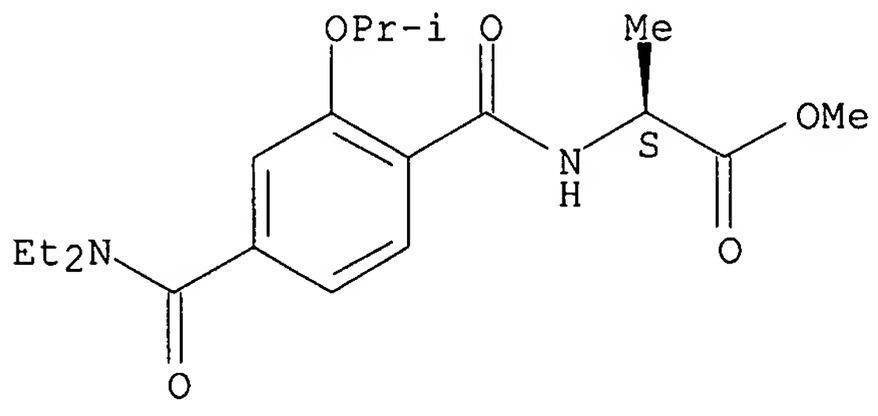
RN 852065-28-2 CAPLUS
CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



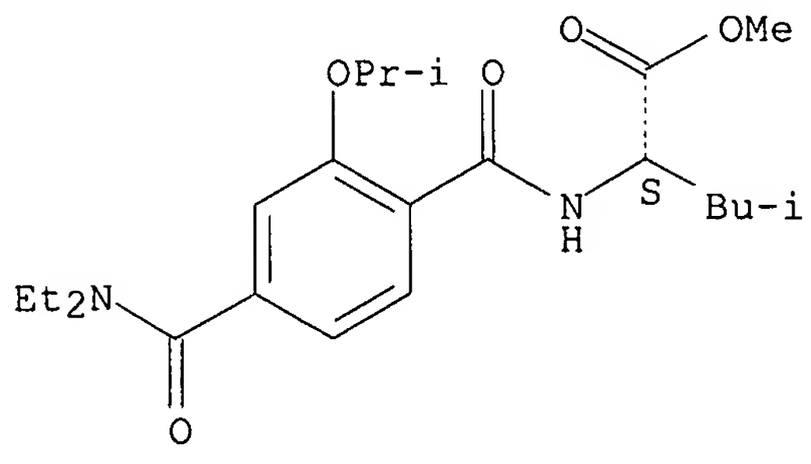
RN 852065-29-3 CAPLUS
CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



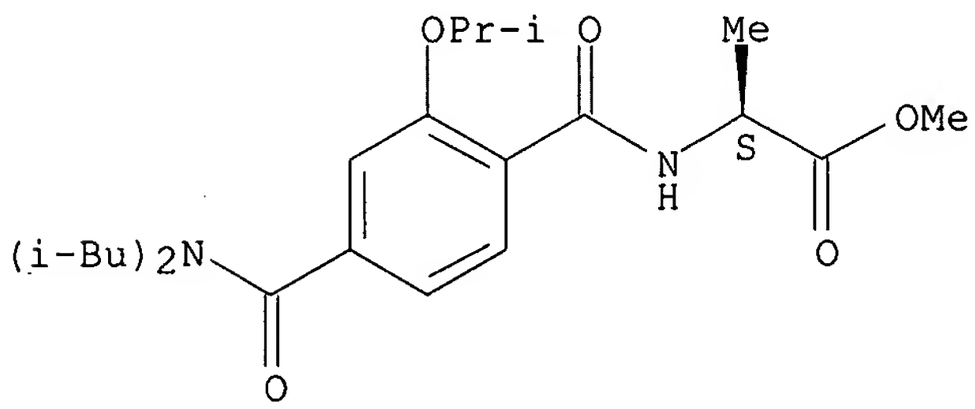
RN 852065-30-6 CAPLUS
CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,
methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



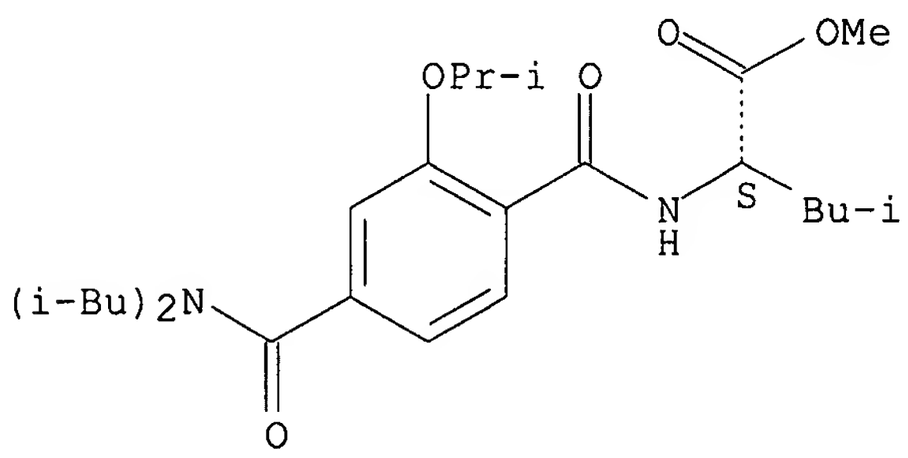
RN 852065-31-7 CAPLUS
CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



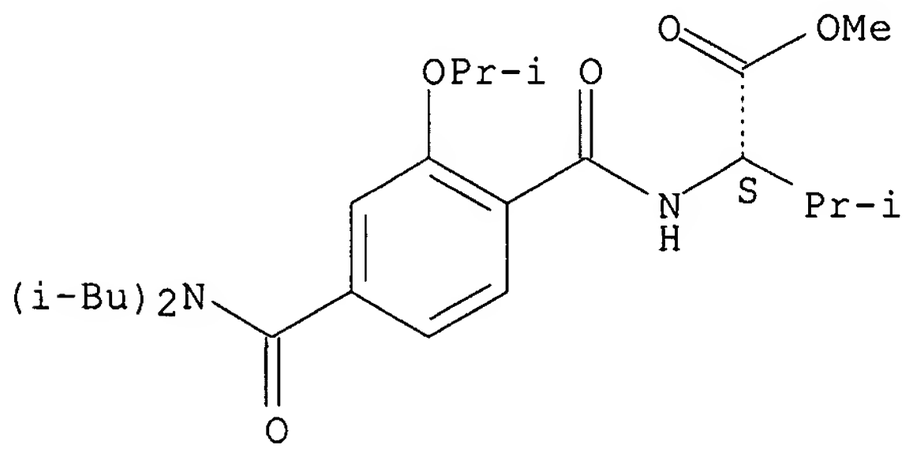

RN 852065-32-8 CAPLUS
CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



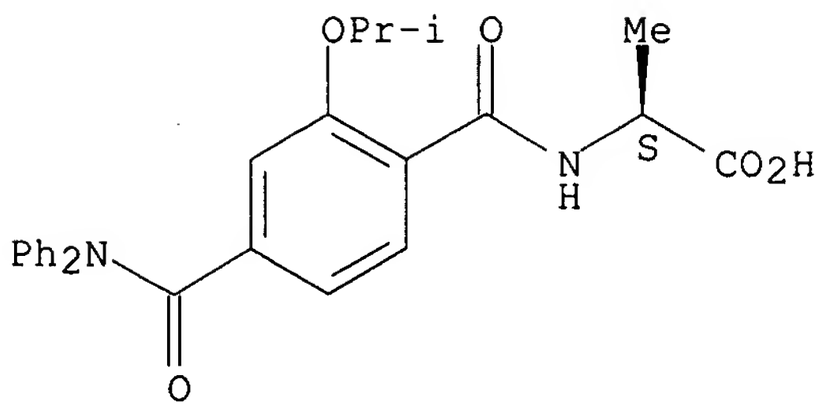

RN 852065-33-9 CAPLUS
CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



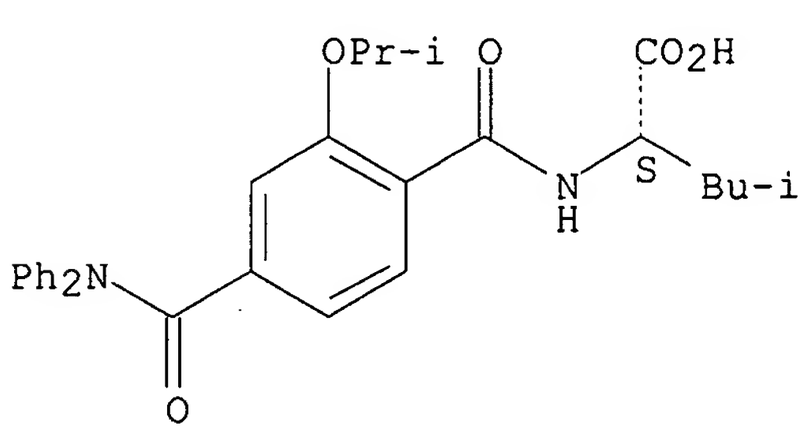

RN 852065-34-0 CAPLUS
CN L-Alanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



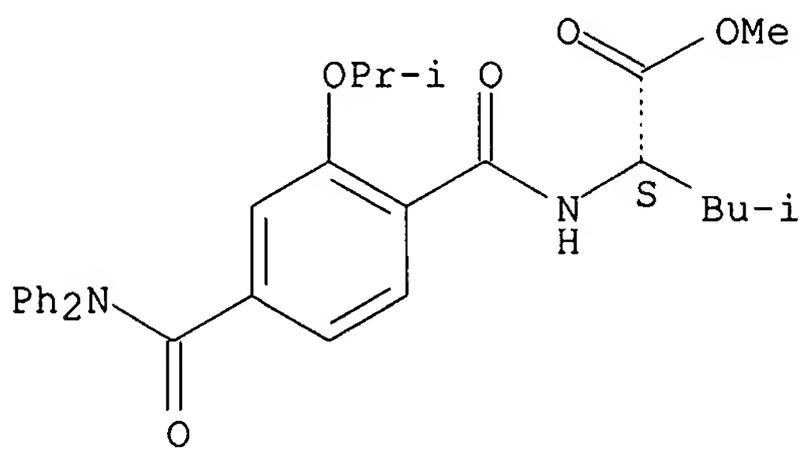
RN 852065-35-1 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



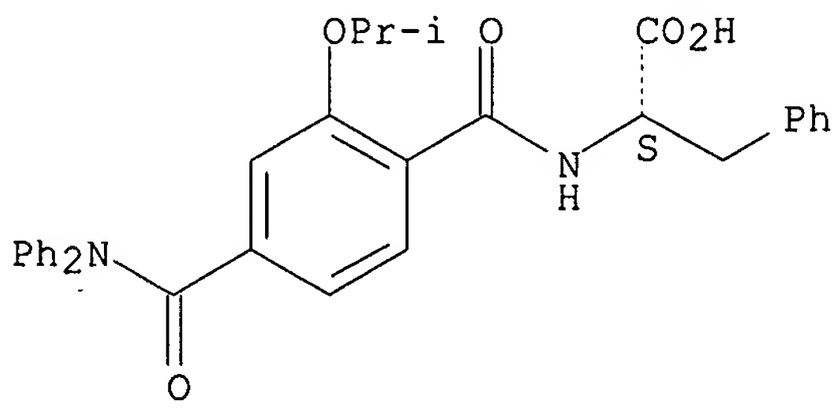
RN 852065-36-2 CAPLUS
CN L-Leucine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 852065-37-3 CAPLUS
CN L-Phenylalanine, N-[4-[(diphenylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



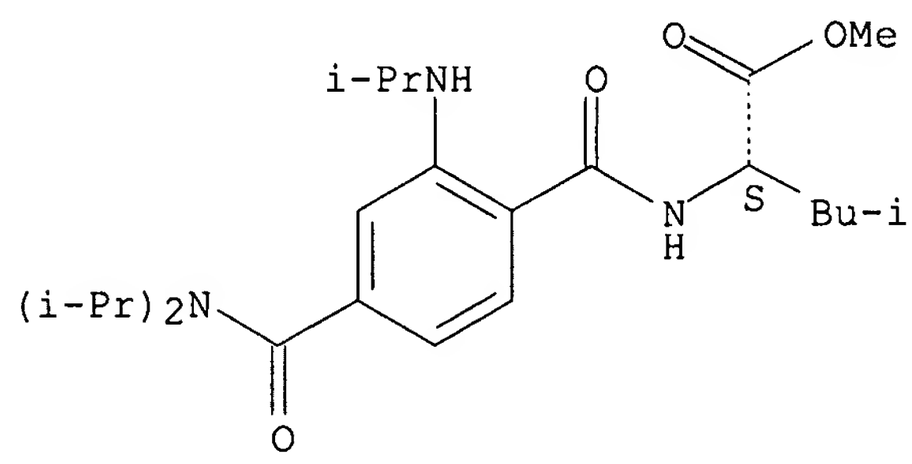
IT 852065-20-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 852065-20-4 CAPLUS

CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.




RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:189140 CAPLUS

DN 140:350050

TI Terephthalamide derivatives as mimetics of the helical region of Bak peptide target Bcl-xL protein

AU Yin, Hang; Hamilton, Andrew D.

CS Department of Chemistry, Yale University, New Haven, CT, 06511, USA

SO Bioorganic & Medicinal Chemistry Letters (2004), 14(6), 1375-1379
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science B.V.

DT Journal

LA English

OS CASREACT 140:350050

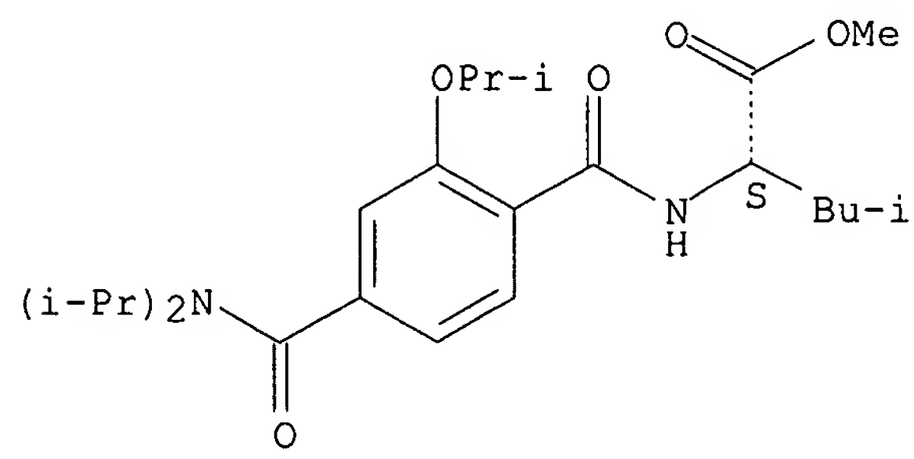
AB A group of novel Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, were designed to mimic the α-helical region of the Bak peptide. Good in vitro inhibition potencies in disrupting the Bak/Bcl-xL complex have been observed (terephthalamide 4, Ki=0.78±0.07 μM).

IT 681465-54-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-54-3 CAPLUS

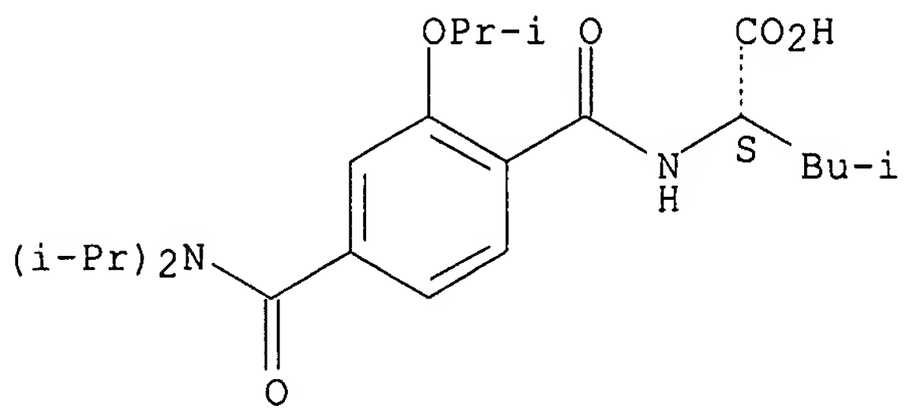
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



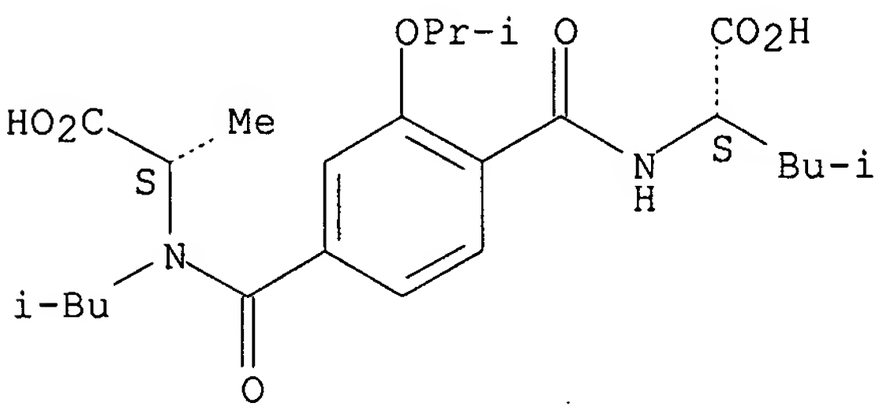
IT 681465-56-5P 681465-58-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)
RN 681465-56-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



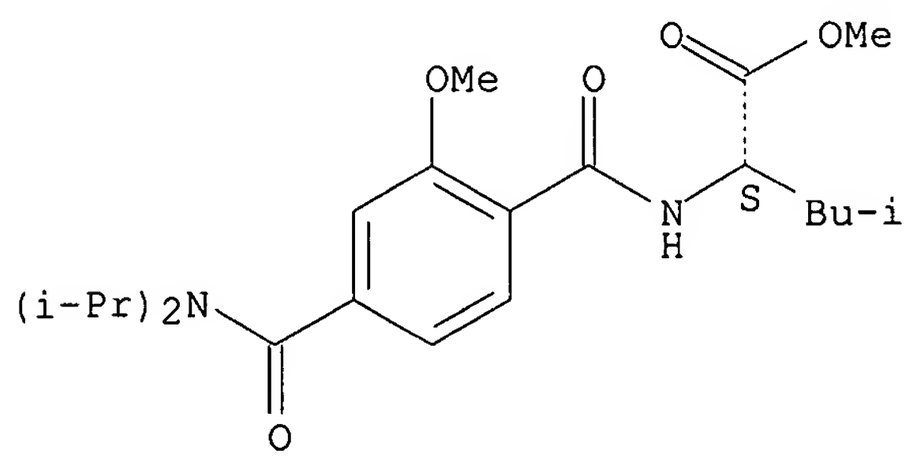

RN 681465-58-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



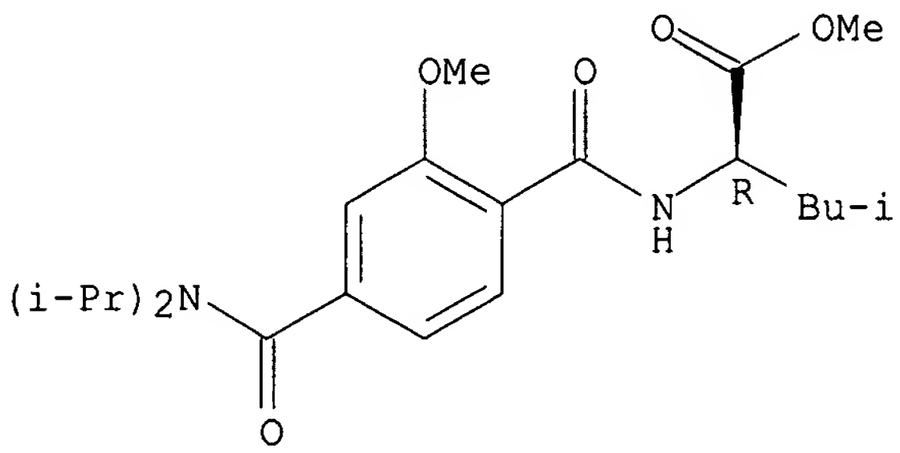

IT 681465-60-1 681465-62-3 681465-64-5
681465-66-7 681465-68-9 681465-70-3
681465-72-5 681465-74-7 681465-80-5
681465-82-7
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)
RN 681465-60-1 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



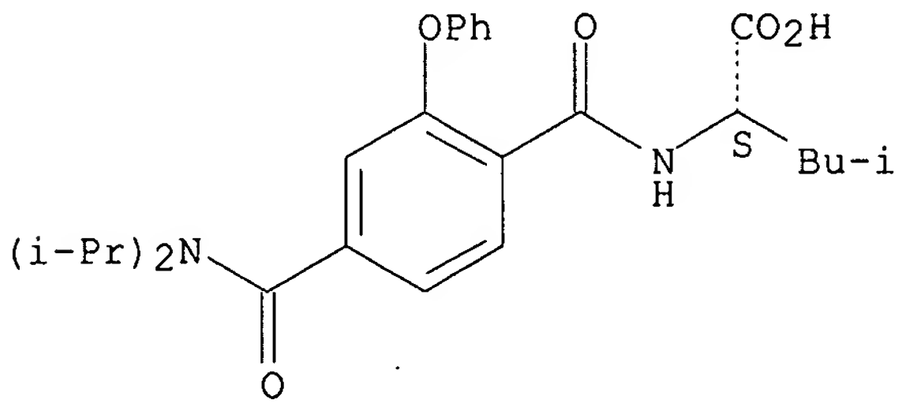
RN 681465-62-3 CAPLUS
CN D-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



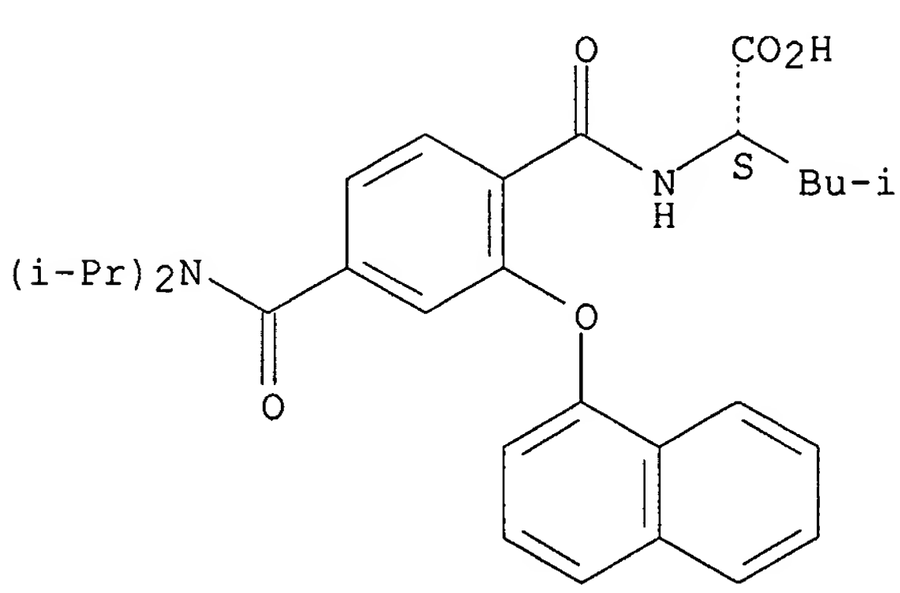

RN 681465-64-5 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



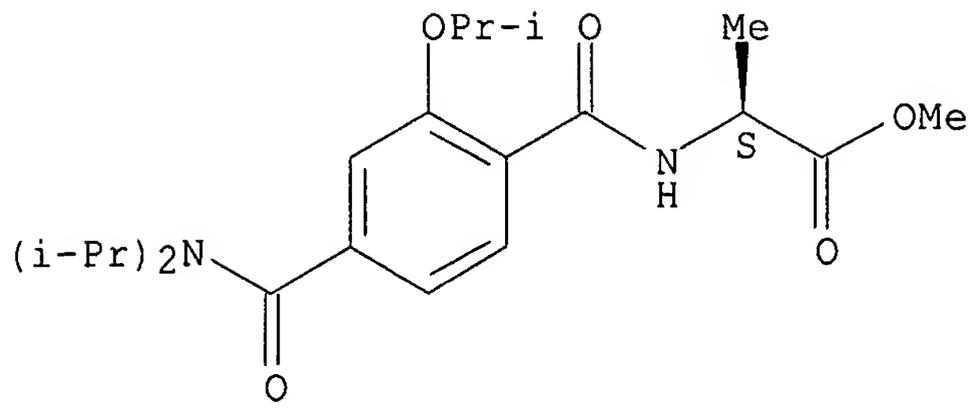

RN 681465-66-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-naphthalenyloxy)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



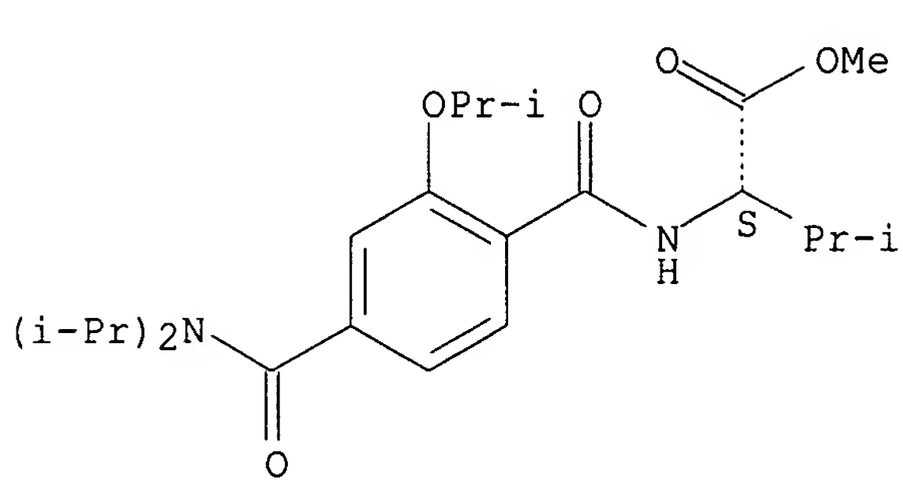

RN 681465-68-9 CAPLUS
CN L-Alanine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



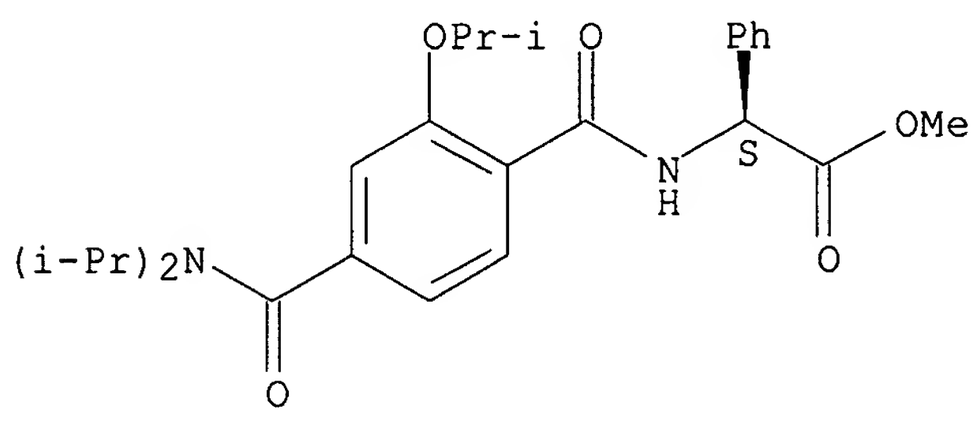
RN 681465-70-3 CAPLUS
CN L-Valine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



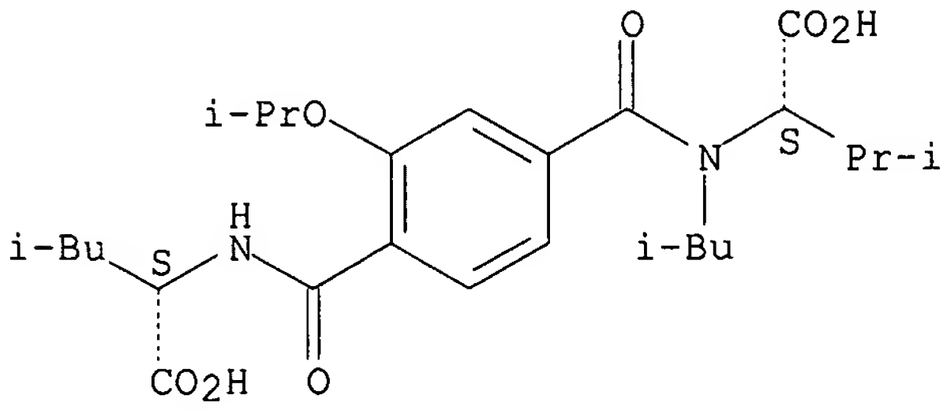
RN 681465-72-5 CAPLUS
CN Benzeneacetic acid, α-[[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]amino]-, methyl ester, (αS)- (CA INDEX NAME)

Absolute stereochemistry.

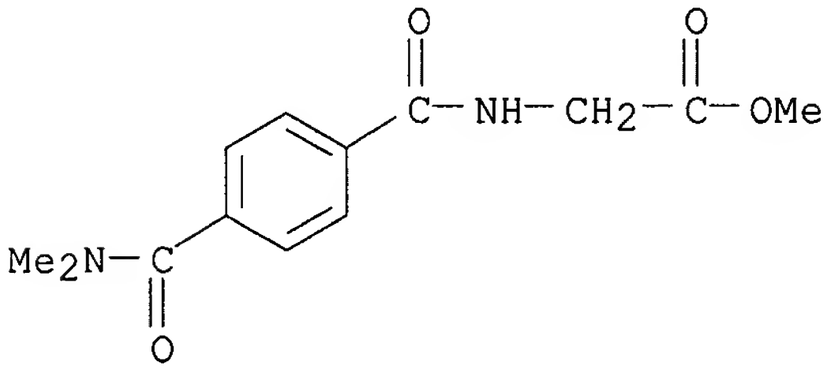


RN 681465-74-7 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

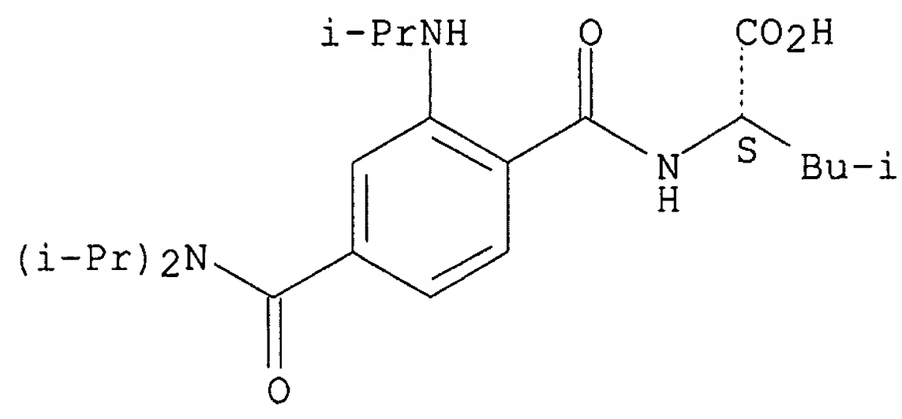


RN 681465-80-5 CAPLUS
CN Glycine, N-[4-[(dimethylamino)carbonyl]benzoyl]-, methyl ester (CA INDEX NAME)



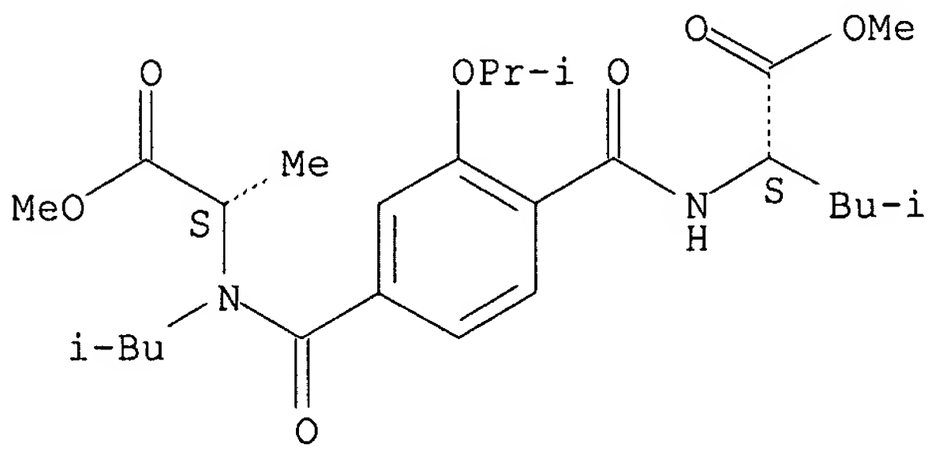
RN 681465-82-7 CAPLUS
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-[(1-methylethyl)amino]benzoyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681466-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)
RN 681466-00-2 CAPLUS
CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

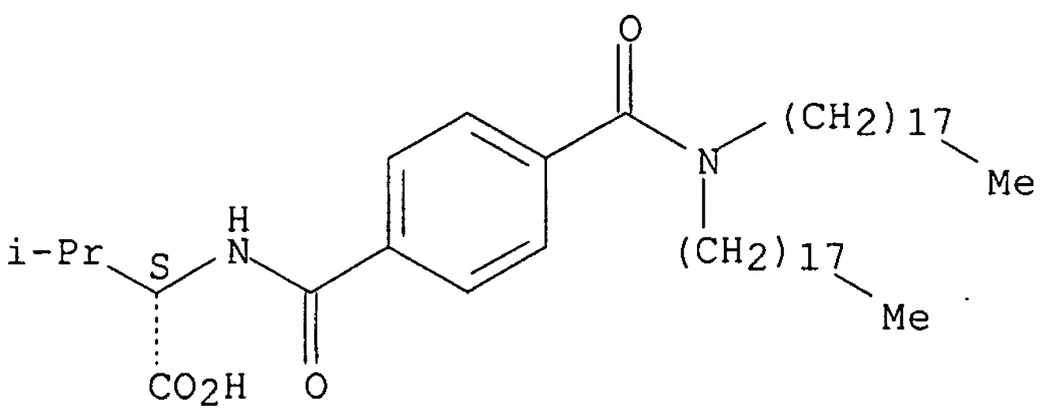


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1999:319884 CAPLUS
DN 131:73949
TI Multisite Recognition of Aqueous Dipeptides by Oligoglycine Arrays Mixed with Guanidinium and Other Receptor Units at the Air-Water Interface
AU Ariga, Katsuhiko; Kamino, Ayumi; Cha, Xiao; Kunitake, Toyoki

CS Supermolecules Project, JST (formerly JRDC), Kurume, 839-0861, Japan
SO Langmuir (1999), 15(11), 3875-3885
CODEN: LANGD5; ISSN: 0743-7463
PB American Chemical Society
DT Journal
LA English
AB Equimolar mixed monolayers of dioctadecyl glycylglycinamide amphiphile (2C18BGly2NH2) with other functional amphiphiles bearing guanidinium, pyridine, and alc. OH groups were prepared on water, and the binding of aqueous dipeptides to these monolayers was investigated by π-A isotherm measurement, FT-IR spectroscopy, and XPS elemental anal. The binding behavior of GlyLeu to the mixed monolayer of 2C18BGly2NH2 and guanidinium amphiphile (2C18BGua) was analyzed by a Langmuir isotherm to give a saturation guest/amphiphile ratio (α) of 0.46 and a binding constant (K) of 6400 M-1. The former value indicates that the binding site for one GlyLeu mol. was formed cooperatively by the two monolayer components. The binding constant is much enhanced relative to those observed for the 2C18BGly2NH2 single-component monolayer (35 M-1) and an equimolar mixed monolayer of 2C18BGly2NH2 and benzoic acid amphiphile (2C18BCOOH) (475 M-1). When the second amphiphile was replaced with a pyridine amphiphile (2C18Py) or with an alc. amphiphile (2C18OH), binding consts. for GlyLeu were lowered to 124 and 43 M-1, resp. The enhanced binding in the former is attributed to strong guanidinium-carboxylate interaction upon C-terminal guest insertion and stable antiparallel hydrogen bonding among peptide chains. The binding of a second dipeptide, LeuGly, to the mixed monolayer of 2C18BGly2NH2/2C18BGua gave a K value (2170 M-1) that is only one-third of that of GlyLeu. The difference is apparently related to the disposition of the hydrophobic side chain of the Leu residue in the C-terminal insertion. Thus, size matching of side chains of amino acid residues in host and guest dets. selectivity of binding. Guest dipeptides are bound to the host most efficiently when the separation of host peptide chains is suited for the formation of strong hydrogen bonds between host and guest.
IT 228713-50-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(multisite recognition of aqueous dipeptides by oligoglycine arrays mixed with guanidinium and other receptor units at air-water interface)
RN 228713-50-6 CAPLUS
CN L-Valine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]- (CA INDEX NAME)

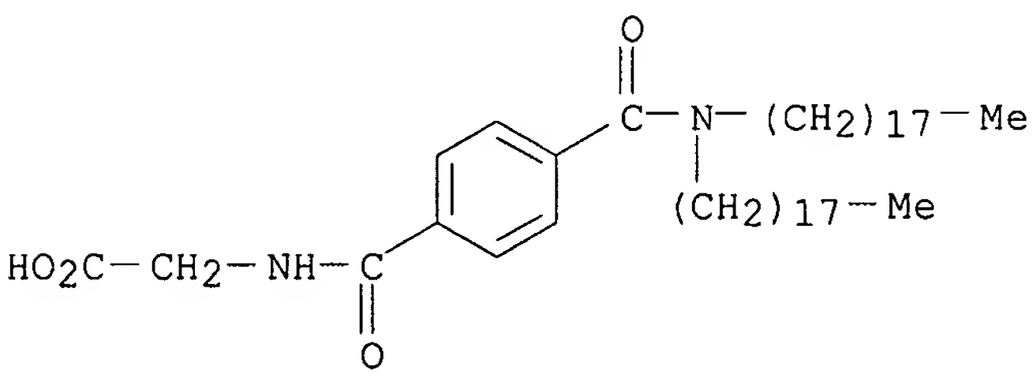
Absolute stereochemistry.




RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

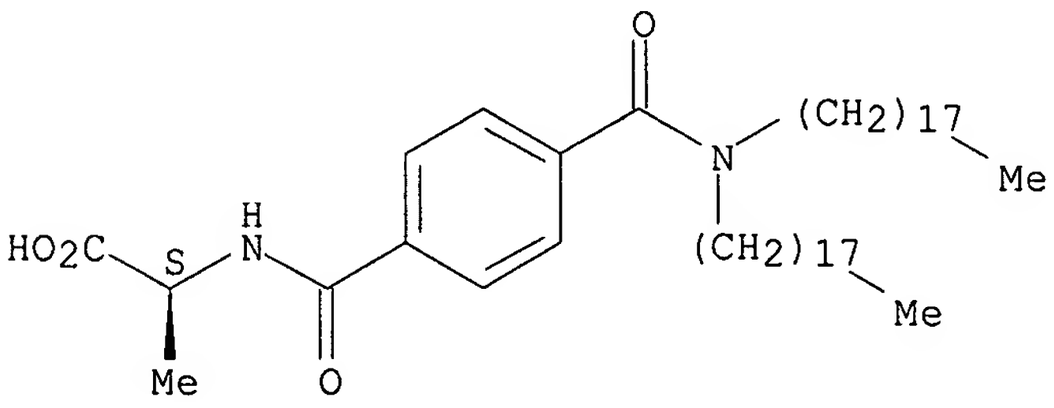
L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
AN 1996:619214 CAPLUS
DN 126:8607
TI Molecular Recognition of Aqueous Dipeptides at Multiple Hydrogen-Bonding Sites of Mixed Peptide Monolayers
AU Cha, Xiao; Ariga, Katsuhiko; Kunitake, Toyoki
CS Supermolecules Project, JRDC, Kurume, 839, Japan
SO Journal of the American Chemical Society (1996), 118(40), 9545-9551

CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB Oligopeptide amphiphiles 4-[Me(CH2)17]2NCOC6H4CO-X-Y-NH2 (I; X = Gly, Ala; Y = Gly, Ala, Val, Leu, Phe) were synthesized. Binding of aqueous dipeptides onto monolayers of equimolar mixts. of these amphiphiles with benzoic acid amphiphile 4-[Me(CH2)17]2NCOC6H4CO2H (II) was investigated by π-A isotherm measurement, FT-IR spectroscopy, and XPS elemental anal. For given dipeptides H-Gly-Z-OH (Z = neutral and hydrophobic residues), the binding ratio was lessened with increasing sizes of the side chain of the Y residue in I. The Langmuir-type saturation behavior was observed for binding of H-Gly-Leu-OH to an equimolar monolayer of I (X = Y = Gly) and II. Its binding constant of 475 M-1 was 10 times larger than that observed for a single-component monolayer of I (X = Y = Gly) (K = 35 M-1). The saturation guest/host ratio was 0.47. The mode of substrate insertion into the binding site was examined by FT-IR spectroscopy. When the hydrophobic residue was on the C-terminal of a guest dipeptide (H-Gly-Z-OH), the C-terminal insertion was selected with accompanying formation of cyclic carboxylic acid dimers at the interface. In the case of H-Z-Gly-OH guests, the N-terminal insertion with salt bridge formation with the host was observed When the two residues of a dipeptide had close hydrophobicities, both C- and N-terminal insertions were observed Formation of these binding sites is apparently induced by dipeptide binding.
IT 183960-45-4P 183960-46-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mol. recognition of aqueous dipeptides at multiple hydrogen-bonding sites of mixed peptide monolayers)
RN 183960-45-4 CAPLUS
CN Glycine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]- (CA INDEX NAME)



RN 183960-46-5 CAPLUS
CN L-Alanine, N-[4-[(dioctadecylamino)carbonyl]benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2             35 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 14:34:02 ON 25 JAN 2008
L3              5 S L2

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| NEWS | 3 AUG 06 | FSTA enhanced with new thesaurus edition |
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| NEWS | 12 SEP 17 | CA/CAplus enhanced with printed CA page images from 1967-1998 |
| NEWS | 13 SEP 17 | CAplus coverage extended to include traditional medicine patents |
| NEWS | 14 SEP 24 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS | 15 OCT 02 | CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt |
| NEWS | 16 OCT 19 | BEILSTEIN updated with new compounds |
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| NEWS | 19 NOV 30 | ICSD reloaded with enhancements |
| NEWS | 20 DEC 04 | LINPADOCDB now available on STN |
| NEWS | 21 DEC 14 | BEILSTEIN pricing structure to change |
| NEWS | 22 DEC 17 | USPATOLD added to additional database clusters |
| NEWS | 23 DEC 17 | IMSDRUGCONF removed from database clusters and STN |
| NEWS | 24 DEC 17 | DGENE now includes more than 10 million sequences |
| NEWS | 25 DEC 17 | TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment |
| NEWS | 26 DEC 17 | MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary |
| NEWS | 27 DEC 17 | CA/CAplus enhanced with new custom IPC display formats |
| NEWS | 28 DEC 17 | STN Viewer enhanced with full-text patent content from USPATOLD |
| NEWS | 29 JAN 02 | STN pricing information for 2008 now available |
| NEWS | 30 JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS | 31 JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS | 32 JAN 28 | MARPAT searching enhanced |
| NEWS | 33 JAN 28 | USGENE timeliness enhanced |
| NEWS | 34 JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS | 35 JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements |

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